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Review of Mass Spectrometry Data from Waste Tank Headspace Analyses

D.S. Sklarew
A.V. Mitroshkov

February 2006

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

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Pacific Northwest National Laboratory
Richland, Washington 99352

Summary

Numerous analytes have been categorized as tentatively identified compounds (TICs) in air samples from the headspaces of the Hanford Site high-level radioactive waste tanks. The tentative identification of these compounds was based mainly on the agreement between the observed mass spectra and a library of published mass spectra with consideration given to the gas chromatographic conditions and retention times. Many of the TICs were found in a limited number of tanks, were identified by only one laboratory or by one method, and/or were thought to be unlikely components of the waste or its degradation products. Consequently, the mass spectra of selected analytes have been reviewed to determine if their tentative identifications were correct. From our current review of 49 TICs, we found 25 that were misidentified and recommend that 54 of the associated results be flagged as suspect and 22 of the associated results be assigned a different compound name.

Acronyms

HASQARD	Hanforrd Analytical Services Quality Assurance Requirements Document
MS	Mass spectra
NHC	Numatec Hanford Company
ORNL	Oak Ridge National Laboratory
PNNL	Pacific Northwest National Laboratory
RT	Retention time
TIC	Tentatively identified compound
TWINS	Tank Waste Information Network System

1.0 Mass Spectral Data Review

Numerous analytes were identified and categorized as tentatively identified compounds (TICs) in air samples from the headspaces of the Hanford Site high-level radioactive waste tanks. The degree of certainty of TIC identification can be highly variable, depending on the philosophy of the analyst and the goal of the analysis. In some cases, the mass spectrum of the unknown matched very closely with the database spectrum, the retention time was reasonable, and there is a high probability the compound (or a close isomer) was correctly identified. In other cases, the identification was based on the "best" computerized match, even though the computer-generated agreement between the unknown and database spectra was less than 60%. Among the latter, there are cases where the unknown has obviously been misidentified.

A recent toxicological review of the more than 1,500 chemicals reported in the tank headspaces identified 72 that needed a detailed toxicological evaluation (Poet et al. 2006). Because a number of these were probably incorrectly identified, an effort has been made to reevaluate the analytical data and flag any misidentified chemicals as suspect in the Tank Waste Information Network System (TWINS 2006) database. Likely candidates were those that have been found in a limited number of tanks, have been identified by only one laboratory or by one method, or were thought to be unlikely components of the waste or its degradation products.

In three previous letter reports (Sklarew and Mitroshkov 2005 a and b; Sklarew and Evans 2005), we reviewed the interpretation of the mass spectra of approximately 165 analytes categorized as TICs in the waste tank headspaces and concluded that 77 of those were incorrectly identified and 37 were correctly identified. We felt there was insufficient evidence to make a definitive identification of many of the remaining TICs, but a conservative approach was taken and these were not classified as suspect.

In this report, we review the interpretation of the mass spectra of 49 additional chemical analytes in waste tank headspace samples categorized as TICs by Oak Ridge National Laboratory (ORNL), Pacific Northwest National Laboratory (PNNL) or Numatec Hanford Company (NHC). Many of these compounds appeared in more than one analysis for an individual tank and several appeared in more than one tank. The reevaluation of analytical data was based on the professional experience and judgment of the authors. In selected cases, guidance was provided by the Hanford Analytical Services Quality Assurance Requirements Document (HASQARD) guidelines[1] (see Appendix A).

Tables 1through 4 summarize our reasoning and conclusions about the validity of the identification of each compound. When a compound was observed in more than one analysis, the spectrum from each analysis was reviewed, except in those cases where the data could not be found or as noted in the tables. In most cases, multiple spectra of an identified compound were very similar and comments made for one analysis apply to all the analyses. An example of the spectrum for each TIC is included in Appendix B in the order listed in the tables (multiple spectra are included if there are significant differences among the spectra for a given TIC). In certain instances, we were able to find an alternative standard mass spectrum that appeared to be a better match with the unknown; these spectra are also included in Appendix B (following the unknown), and the proposed identifications are specified in the table.

[1] The HASQARD requirements were provided by Dr. Mark Marcus via email.

We have divided the analytes considered into four categories. The first category includes those analytes that have good to excellent mass spectral fits and appear to have reasonable retention times. We concur with the original identification of these analytes, though in some cases it could not be determined whether the specific isomer named was correct. Also included in this category are analytes that have reasonable mass spectral fits if they are considered as part of a mixture. These are listed in Table 1 with selected analytical data and comments.

The second category includes those analytes we consider to be misidentified and for which we are recommending that the analyte name be changed. The analyte name changes are based on significantly better mass spectral matches and/or retention times. These are listed in Table 2 with selected analytical data, the recommended name change, and comments.

Analytes that in our opinion were misidentified and for which we have no recommended name change constitute the third category. Our conclusion is most often based on poor agreement between the observed and library mass spectra; but in some cases, the retention time is not compatible with the identification. These analytes are listed in Table 3 with selected analytical data and comments. Included in this category are those analytes that, in our opinion, were likely misidentified based on the spectral and chromatographic evidence, but that we could not definitively state to be incorrect. Of these analytes, the ones that failed the HASQARD guidelines (see Appendix A) are included in this category and noted in the comments section of Table 3.

The fourth category includes 14 analytical results for which we were unable to locate the mass spectral data. These are listed in Table 4.

Based on our review, we recommend treating 54 of the reported results associated with 21 analytes as suspect on the basis that they were misidentified. We concur with 56 of the reported results associated with 19 analytes in Table 1 and recommend name changes for 22 reported results associated with six analytes in Table 2.

2.0 References

Poet, TS, TJ Mast, and JL Huckaby. 2006. Screening Values for Non-Carcinogenic Hanford Waste Tank Vapor Chemicals that Lack Established Occupational Exposure Limits. PNNL-15640 rev 0. Pacific Northwest National Laboratory, Richland, Washington.

Sklarew DS and AV Mitroshkov. 2005. Review of ORNL Mass Spectrometry Data from Waste Tank Headspace Analyses. Letter report to Jim Honeyman, TWS05.008 rev 1. March 2005.

Sklarew DS and AV Mitroshkov. 2005. Review of ORNL Mass Spectrometry Data from Waste Tank Headspace Analyses. Letter report to Jim Honeyman, TWS05.016. April 2005.

Sklarew DS and JC Evans. 2005. Review of PNNL Mass Spectrometry Data from Waste Tank Headspace Analyses. Letter report to Jim Honey, TWS05.021. September 2005.

TWINS 2006. Tank Waste Information Network System. http://twins.pnl.gov.

Table 1. Confirmed Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Retention Time Reference	Comments
BY-108	36653-82-4	1-Hexadecanol	S4076-A10.649		86.33[(b)]	pentadecanoic acid RT 89.68; hexadecane RT 78.74	MS - reasonable, but hard to say; RT - ok?
C-103	36653-82-4	1-Hexadecanol	S4025-D20.352		90.90[(a)]	pentadecanoic acid RT 85.41; hexadecane RT 75.68	MS - scan doesn't go to high enough m/e; RT - ok?
B-103	1115-11-3	2-Butenal, 2-methyl-	S6114-m28.1027		22.46[(a)]	1-butanol RT 22.2	RT - reasonable; MS - good fit, but could be isomer such as 2-ethylacrolein or 2-pentenal
B-103	1115-11-3	2-Butenal, 2-methyl-	S6115-m28.1013		22.61[(a)]	1-butanol RT 22.3	RT - reasonable; MS - good fit, but could be isomer such as 2-ethylacrolein or 2-pentenal
B-103	1115-11-3	2-Butenal, 2-methyl-	S6114-b36.1031				assume this is the same as the others
B-103	1115-11-3	2-Butenal, 2-methyl-	S6114-t44.1037		22.49[(a)]	1-butanol RT 22.2	RT - reasonable; MS - good fit, but could be isomer such as 2-ethylacrolein or 2-pentenal
B-103	1115-11-3	2-Butenal, 2-methyl-	S6115-t45.1053				assume this is the same as the others
B-103	1115-11-3	2-Butenal, 2-methyl-	S6115-t44.1073		22.48[(a)]	1-butanol RT 22.2	RT - reasonable; MS - good fit, but could be isomer such as 2-ethylacrolein or 2-pentenal
B-103	1115-11-3	2-Butenal, 2-methyl-	S6114-m49.1048				assume this is the same as the others
C-105	51595-87-0	2-Heptanone, 6-(2-furanyl)-6-methyl-	S4005-41.B16		67.08[(b)]	C14-alkane RT 66.64	MS - reasonably good fit; RT ok
C-105	51595-87-0	2-Heptanone, 6-(2-furanyl)-6-methyl-	S4005-42.B16		67.08[(b)]	C14-alkane RT 66.64	MS - reasonably good fit; RT ok
C-103	928-68-7	2-Heptanone, 6-methyl-	S4025-D03.342		45.27[(b)]	d5-bromobenzene RT 43.98; nonane RT 41.40	MS - reasonable; RT reasonable
C-103	928-68-7	2-Heptanone, 6-methyl-	S4025-D19.347		45.25[(b)]	d5-bromobenzene RT 43.98; nonane RT 41.43	MS - reasonable; RT reasonable
C-103	928-68-7	2-Heptanone, 6-methyl-	S4025-D18.325		45.21[(b)]	d5-bromobenzene RT 43.95; nonane RT 41.37	MS - reasonable; RT reasonable
C-103	928-68-7	2-Heptanone, 6-methyl-	S4025-D20.352		45.26[(b)]	d5-bromobenzene RT 43.97; nonane RT 41.39	MS - reasonable; RT reasonable
C-103	928-68-7	2-Heptanone, 6-methyl-	S4025-D02.285		40.34[(c)]	d5-bromobenzene RT 39.01; nonane RT 36.40	MS - reasonable; RT reasonable (diff GC program than others)
C-103	105-42-0	2-Hexanone, 4-methyl-	S4025-D02.285		32.87[(c)]	d5-bromobenzene RT 43.98; nonane RT 41.40	MS - reasonable; RT reasonable
AX-102	645-62-5	2-Hexenal, 2-ethyl-	S5035-A14.813		50.45[(a)]	ethylbenzene-d10 RT 41.52	MS - possible; RT - ok?

Table 1. Confirmed Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Retention Time Reference	Comments
AX-102	645-62-5	2-Hexenal, 2-ethyl-	S5035-A12.1003		50.44[(a)]	ethylbenzene-d10 RT 41.48; 4-octanone RT 48.59	MS - possible; RT - ok?
AX-102	645-62-5	2-Hexenal, 2-ethyl-	S5035-A13.1004		50.44[(a)]	ethylbenzene-d10 RT 41.47; 4-octanone RT 48.59	MS - possible; RT - ok?
BY-104	814-78-8	3-Buten-2-one, 3-methyl-	S4019-A13.250		19.17[(d)]	d6-benzene RT 17.67; heptane RT 21.24	MS - possible; RT - ok?
C-103	589-38-8	3-Hexanone	S4025-D04.345		33.07[(b)]	toluene-d8 RT 31.27; octane 34.06	MS - good fit; RT reasonable (could be isomer)
C-103	589-38-8	3-Hexanone	S4025-D09.290		32.79[(b)]	toluene-d8 RT 30.95; octane 33.76	MS - good fit; RT reasonable (could be isomer)
C-103	589-38-8	3-Hexanone	S4025-D10.364		32.85[(b)]	toluene-d8 RT 31.01; octane 33.82	MS - good fit; RT reasonable (could be isomer)
C-103	589-38-8	3-Hexanone	S4025-D11.366		32.78[(b)]	toluene-d8 RT 30.94; octane 33.75	MS - good fit; RT reasonable (could be isomer)
C-103	589-38-8	3-Hexanone	S4025-D02.285		28.24[(c)]	toluene-d8 RT 26.40; octane 29.10	MS - good fit; RT reasonable (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D03.342		74.27[(b)]	d26-dodecane RT 59.02	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D05.358		74.32[(b)]	d26-dodecane RT 59.07; tetradecane RT 70.09	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D04.345		74.30[(b)]	d26-dodecane RT 59.10; tetradecane RT 70.07	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D10.364		74.01[(b)]	d26-dodecane RT 58.78; tetradecane RT 69.78	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D11.366		73.84[(b)]	d26-dodecane RT 58.67; tetradecane RT 69.65	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D19.347		74.29[(b)]	d26-dodecane RT 59.03; tetradecane RT 70.09	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D18.325		74.26[(b)]	d26-dodecane RT 59.06; tetradecane RT 70.05	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D20.352		74.31[(b)]	d26-dodecane RT 59.08; tetradecane RT 70.10	MS - reasonable; RT - ok? (could be isomer)
C-103	1534-26-5	3-Tridecanone	S4025-D02.285		69.40[(c)]	pentadecane? 69.63	MS - reasonable; RT - ok? (could be isomer)

Table 1. Confirmed Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Retention Time Reference	Comments
C-103	UHC000-13M	C2-Pyridine and others	S4025-D09.290		49.06[(b)]	d5-bromobenzene RT 43.76; decane RT 47.90	MS- mixture but reasonable (would help to have raw data to determine which peaks match up); RT - long? - but consistent with dimethylpyridine RT in this table
BY-104	625-86-5	Furan, 2,5-dimethyl-	S4019-A12.249		26.11[(b)]	d6-benzene RT 21.73; heptane RT 25.31	MS - good fit; RT - reasonable
AX-102	1703-52-2	Furan, 2-ethyl-5-methyl-	S5035-A13.1004		37.30[(a)]	ethylbenzene-d10 RT 41.47	MS - possible; RT - ok?
BY-104	1703-52-2	Furan, 2-ethyl-5-methyl-	S4019-A12.249		33.63[(b)]	ethylbenzene-d10 RT 37.90	MS - possible; RT - ok?
BY-104	534-22-5	Furan, 2-methyl-	S4019-A12.249		16.76[(b)]	hexafluorobenzene RT 17.61; hexane RT 16.13; 2-butanone RT 16.36	MS - good fit; RT reasonable?
C-103	534-22-5	Furan, 2-methyl-	S4025-D02.285		12.72[(c)]	hexafluorobenzene RT 13.58; hexane RT 12.10	MS - possible, some ratios poor, but probably mixture; RT?
AX-101	3777-69-3	Furan, 2-pentyl-	S5028-A14.978		49.84[(a)]	ethylbenzene-d10 RT 41.52; 3-heptanone RT 43.22; dodecane-d26 RT 60.01	MS - pretty good fit; ratios a little different, but reasonable; RT - possible
AX-101	3777-69-3	Furan, 2-pentyl-	S5028-A13.977		49.84[(a)]	ethylbenzene-d10 RT 41.57; 3-heptanone RT 43.24; dodecane-d26 RT 59.99	MS - pretty good fit; ratios a little different, but reasonable; RT - possible
AX-101	3777-69-3	Furan, 2-pentyl-	S5028-A12.976		49.82[(a)]	ethylbenzene-d10 RT 41.53; 3-heptanone RT 43.21; dodecane-d26 RT 59.97	MS - pretty good fit; ratios a little different, but reasonable; RT - possible
AX-103	3777-69-3M	Furan, 2-pentyl- and others	S5029-A19.995		49.83[(a)]	ethylbenzene-d10 RT 41.50; dodecane-d26 RT 59.97	MS - pretty good fit; ratios a little different, but reasonable (peak at m/e 99 doesn't correspond to peak at m/e 81); RT - possible
C-103	UHC000-09	Methyl pyridine	S4025-D02.285		30.85[(c)]	d10-ethylbenzene RT 33.59; octane RT 29.10	MS-good fit; RT reasonable
C-103	108-47-4	Pyridine, 2,4-dimethyl-	S4025-D02.285		44.03[(c)]	d5-bromobenzene RT 39.01; decane RT 43.13	MS - good fit; RT reasonable, but cf to 30.85 for methylpyridine?
BY-107	1184-60-7	1-Propene, 2-fluoro-	S4077-A16.625	1	12.08[(b)]	hexafluorobenzene RT 15.99; d2-methylene chloride RT 8.99; hexane RT 14.50	MS - possible, possible mixture with cyclopropene; RT - too long?

Table 1. Confirmed Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Retention Time Reference	Comments
BY-107	1184-60-7	1-Propene, 2-fluoro-	S4077-A17.785	1	12.31[(b)]	hexafluorobenzene RT 16.13; d2-methylene chloride RT 9.13; hexane RT 14.63	MS - possible, possible mixture with cyclopropene; RT - too long?
BY-107	1184-60-7	1-Propene, 2-fluoro-	S4077-A18.632	1	12.29[(b)]	hexafluorobenzene RT 16.12; d2-methylene chloride RT 9.16; hexane RT 14.64	MS - possible, possible mixture with cyclopropene; RT - too long?
BY-108	1184-60-7	1-Propene, 2-fluoro-	S4076-A14.855	1	12.26[(b)]	hexafluorobenzene RT 16.08; d2-methylene chloride RT 9.04	MS - possible, possible mixture with cyclopropene; RT - too long?
C-105	1184-60-7	1-Propene, 2-fluoro-	S4005-41.B16	1	13.11[(b)]	2-propanone RT 7.29	MS - possible, possible mixture with cyclopropene; RT - too long?
TY-104	1184-60-7	1-Propene, 2-fluoro-	S4063-03.328	1	12.83[(a)]	hexafluorobenzene RT 16.82; d2-methylene chloride RT 9.62; (no hexane)	MS - possible, possible mixture with cyclopropene; RT - too long?
C-107	1184-60-7M	1-Propene, 2-fluoro- and others	S4058-A15.701	1	11.94[(b)]	hexafluorobenzene RT 15.88; d2-methylene chloride RT 8.78; (no hexane)	MS - possible, possible mixture with cyclopropene; RT - too long?
BY-106	109-75-1	3-Butenenitrile	S4021-A11.293	1	21.10[(b)]	hexane RT 16.01; hexafluorobenzene RT 17.46; d6-benzene RT 21.63	MS - reasonable, if mixture; RT could be ok
AX-102	34379-54-9	Furan, 2,3-dihydro-4-(1-methylpropyl)-, (S)-	S5035-A12.1003	1	44.82[(a)]	ethylbenzene-d10 RT 41.48	MS - possible; RT - ok?; part of a mixture

1 Identification is reasonable if the mass spectrum is considered to consist of a mixture of the specified analyte and some other unnamed analyte.

(a) Gas chromatograph column conditions not available.

(b) Gas chromatograph held at 10 °C for 10 minutes, ramped to 230 °C at 3 °C per minute, held at 230 °C for 16.7 min.

(c) Gas chromatograph held at 10 °C for 5 minutes, ramped to 230 °C at 3 °C per minute., held at 230 °C for 16.7 min.

(d) Gas chromatograph held at 10 °C for 6 minutes, ramped to 230 °C at 3 °C per minute, held at 230 °C for 16.7 min..

Table 2. Misidentified Analytes with Recommended Name Changes

Tank	Chemical Id	Existing Analyte Name	Field Sample Id	Retention Time	Reference Retention Time	Recommended Analyte Name	Comments
AX-102	3457-91-8	1,4-Butanediol, dinitrate	S5035-A14.813	38.99[(a)]	ethylbenzene-d10 41.52	Nitric acid, butyl ester	MS - ok, but nitric acid, butyl ester is better fit; RT too short
AX-102	3457-91-8	1,4-Butanediol, dinitrate	S5035-A13.1004	31.44 & 38.93[(a)]	benzene-d6 RT 25.98	Nitric acid, propyl ester and Nitric acid, butyl ester	MS - ok, but nitric acid, propyl ester is better fit at 31.44 RT and nitric acid, butyl ester is better fit at 38.93 RT; RT too short
AX-102	3457-91-8	1,4-Butanediol, dinitrate	S5035-A12.1003	38.97[(a)]	ethylbenzene-d10 41.48	Nitric acid, butyl ester	MS - ok, but nitric acid, butyl ester is better fit; RT too short
AX-103	3457-91-8	1,4-Butanediol, dinitrate	S5029-A16.993	31.57[(a)]	benzene-d6 RT 26.15; nitromethane 17.92; 3-heptanone RT 43.22	Nitric acid, propyl ester	MS - ok, but nitric acid, propyl ester is better fit; RT too short
BY-107	3457-91-8	1,4-Butanediol, dinitrate	S4077-A18.632	33.85[(b)]	toluene-d8 RT 29.13; octane RT 31.92	Nitric acid, butyl ester	MS - ok, but nitric acid, butyl ester is better fit; RT too short
C-103	3457-91-8	1,4-Butanediol, dinitrate	S4025-D02.285	23.22[(c)]	d5-bromobenzene RT 43.98; nonane RT 41.40	Nitric acid, propyl ester	MS - ok, but nitric acid, propyl ester is better fit; GC program different than others; RT too short
TX-106	623-87-0	1,3-Dinitrate-1,2,3-propanetriol	V7012-A04-031	25.36[(a)]	2-butanone 20.77; 1-butanol 23.57	Nitric acid, propyl ester	MS fit not very good (peak ratios not quite right, no m/e 73 or 45, and 60 is less, but these are all small); RT too short; nitric acid, propyl ester is better fit
TX-108	623-87-0	1,3-Dinitrate-1,2,3-propanetriol	V7043-A04-065	25.79[(a)]	2-butanone 20.39; 1-butanol 23.21	Nitric acid, propyl ester	MS fit not very good (peak ratios not quite right, no m/e 73 or 45, and 60 is less, but these are all small); RT too short; nitric acid propyl ester is better fit
B-103	3457-92-9	1,5-Pentanediol, dinitrate	S5003-A15.741	45.01[(a)]	ethylbenzene-d10 RT 40.79; benzene-d6 RT 25.39; 3-heptanone RT 42.53	Nitric acid, pentyl ester	note that nitric acid propyl ester is identified at RT 30.84;nitric acid butyl ester is ID'd at RT 38.30; MS- not good fit, m/e 46/76 ratio wrong, no m/e 55 or 85; RT?; 1-butanol, 3-methyl-, nitrate or pentyl nitrate is much better fit
B-103	3457-92-9	1,5-Pentanediol, dinitrate	S5003-A17.383	45.04[(a)]	ethylbenzene-d10 RT 40.83; benzene-d6 RT 25.51; 3-heptanone RT 42.57	Nitric acid, pentyl ester	note that nitric acid propyl ester is identified at RT 30.92; nitric acid butyl ester is ID'd at RT 38.35; MS- not good fit, m/e 46/76 ratio wrong, no m/e 55 or 85; RT?; 1-butanol, 3-methyl-, nitrate or pentyl nitrate is much better fit

Table 2. Misidentified Analytes with Recommended Name Changes

Tank	Chemical Id	Existing Analyte Name	Field Sample Id	Retention Time	Reference Retention Time	Recommended Analyte Name	Comments
B-103	3457-92-9	1,5-Pentanediol, dinitrate	S5003-A16.424	45.00[a]	ethylbenzene-d10 RT 40.77; benzene-d6 RT 25.19; 3-heptanone RT 42.52	Nitric acid, pentyl ester	note that nitric acid propyl ester is identified at RT 30.72; nitric acid butyl ester is ID'd at RT 38.26; MS- not good fit, m/e 46/76 ratio wrong, no m/e 55 or 85; RT?; nitric acid, pentyl ester is better fit
C-105	3457-92-9	1,5-Pentanediol, dinitrate	S4005-41.B16	42.00[b]	butanoic acid, butyl ester RT 46.52; d5-bromobenzene RT 42.67	Nitric acid, pentyl ester	MS - not very good; RT - too short; nitric acid, pentyl ester is better fit
C-107	3457-92-9	1,5-Pentanediol, dinitrate	S4058-A16.784	40.91[b]	nonane RT 39.04	Nitric acid, pentyl ester	MS - not very good; RT - too short; nitric acid, pentyl ester is better fit
C-107	3457-92-9	1,5-Pentanediol, dinitrate	S4058-A15.701	40.91[b]	nonane RT 39.06; d-bromobenzene RT 41.53	Nitric acid, pentyl ester	MS - not very good; RT - too short; nitric acid, pentyl ester is better fit
C-107	3457-92-9	1,5-Pentanediol, dinitrate	S4058-A19.810	40.91[b]	nonane RT 39.04; d-bromobenzene RT 41.51	Nitric acid, pentyl ester	MS - not very good; RT - too short; nitric acid, pentyl ester is better fit
TY-104	3457-92-9	1,5-Pentanediol, dinitrate	S4063-01.314	41.76[b]	nonane RT 39.91; d-bromobenzene RT 42.40	Nitric acid, pentyl ester	MS - not very good; RT - too short; nitric acid, pentyl ester is better fit
TY-104	3457-92-9	1,5-Pentanediol, dinitrate	S4063-03.328	41.72[a]	nonane RT 39.90; d-bromobenzene RT 42.39	Nitric acid, pentyl ester	MS - not very good; RT - too short; nitric acid, pentyl ester is better fit
BY-108	112-92-5	1-Octadecanol	S4076-A10.649	69.93[a]	pentadecane RT 67.87 or 71.66; pentadecanoic acid RT 85.41	Unknown alcohol	MS - scan doesn't go to high enough m/e; RT - too short; possibly lower MW alcohol
BY-106	1708-29-8	Furan, 2,5-dihydro-	S4021-A13.304	21.24[b]	d6-benzene RT 21.73; 2-methylhexane RT 22.35; 2-propylfuran RT 22.13	2-Butenal	MS - 41/42 ratio is wrong, 2-butenal better fit; RT - long?(cfd to 2-propylfuran)
BY-106	1708-29-8	Furan, 2,5-dihydro-	S4021-A12.300	21.10[b]	d6-benzene RT 21.58; 2-methylhexane RT 22.20; 2-propylfuran RT 22.99	2-Butenal	MS - 41/42 ratio is wrong, 2-butenal better fit; RT - long?(cfd to 2-propylfuran)
C-103	1708-29-8	Furan, 2,5-dihydro-	S4025-D02.285	17.05[c]	hexafluorobenzene RT 13.58; heptane 21.04	2-Butenal	MS - 41/42 ratio is wrong, 2-butenal better fit; RT - ok? Or long?

Table 2. Misidentified Analytes with Recommended Name Changes

Tank	Chemical Id	Existing Analyte Name	Field Sample Id	Retention Time	Reference Retention Time	Recommended Analyte Name	Comments
U-106	694-05-3	Pyridine, 1,2,3,6-tetrahydro-	S5012-A15.526			Pyrazine	can't find compound in data package; analyte was apparently mislabeled in report at RT 32.03 but labeled as pyrazine in MS data package; pyrazine is good MS fit

(a) Gas chromatograph column conditions not available.
(b) Gas chromatograph held at 10 °C for 10 minutes, ramped to 230 °C at 3 °C per minute, held at 230 °C for 16.7 min.
(c) Gas chromatograph held at 10 °C for 5 minutes, ramped to 230 °C at 3 °C per minute., held at 230 °C for 16.7 min.

Table 3. Misidentified Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Reference Retention Time Comparison	Comments
AX-102	1192-51-4	2,4(3H,5H)-Furandione, 3-methyl-	S5035-A14.813		60.49[a]	dodecane-d26 RT 59.97	MS - poor match, 113/114 ratio wrong; RT too long
AX-102	1192-51-4	2,4(3H,5H)-Furandione, 3-methyl-	S5035-A12.1003		60.46[a]	dodecane-d26 RT 59.98	MS - poor match, 113/114 ratio wrong; RT too long
AX-102	1192-51-4	2,4(3H,5H)-Furandione, 3-methyl-	S5035-A13.1004		60.49[a]	dodecane-d26 RT 59.93	MS - poor match, 113/114 ratio wrong; RT too long
U-112	1615-70-9	2,4-Pentadienenitrile	S6118-b30.103	1	20.69[a]	heptane 19.26; toluene 22.6	RT - too long; MS not very good fit; didn't scan far enough; doesn't meet HASQARD criteria
C-102	20474-93-5M	2-Butenoic acid, 2-propenyl ester and others	S4057-A13.435	2	61.62[b]	dimethyldodecane RT 61.53	MS - poor fit; RT too long; more likely a cycloalkane
SX-106	717-21-5	2-Propen-1-one, 3-(2-furanyl)-1-phenyl-	S5018-A12.496		81.15[a]	tetradecane - RT 69.45	MS - poor fit, no m/e 197, 105, 121, 65
C-103	616-45-5	2-Pyrrolidinone	S4025-D02.285		33.34[c]	methylpyridine RT 30.85	MS - poor fit; RT too long
BY-108	627-27-0	3-Buten-1-ol	S4076-A14.855		6.00[b]	d2-methylene chloride RT 9.04; 2-propanol? RT 7.45	MS - ratios not very good, doesn't appear to have m/e 53 or 54, but page is too washed out; RT too short?
BY-107	31681-26-2	alpha-Propyl-2-furanacetaldehyde	S4077-A17.785	1,2	48.05[b]	d5-bromobenzene RT 39.72; undecane RT 49.46; d26-dodecane RT 54.00	MS- possible but not likely (mixture); RT -ok?; more likely a branched alkene; doesn't meet HASQARD criteria
BY-107	31681-26-2	alpha-Propyl-2-furanacetaldehyde	S4077-A16-625	1,2	50.45[b]	d5-bromobenzene RT 41.63; undecane RT 51.95; d26-dodecane RT 56.59	MS- possible but not likely (mixture); RT -ok?; more likely a branched alkene; doesn't meet HASQARD criteria
A-101	2549-67-9	Aziridine, 2-ethyl-	S5026-A14.960		37.61[a]	ethylbenzene-d10 RT 42.00; 4-heptanone RT 42.76	MS - not available (MS found by AVM - poor fit); RT - too long
A-101	2549-67-9	Aziridine, 2-ethyl-	S5026-A13.846		37.49[a]	ethylbenzene-d10 RT 41.95; 4-heptanone RT 42.72	MS - not available (MS found by AVM - poor fit); RT - too long
A-101	2549-67-9	Aziridine, 2-ethyl-	S5026-A12.823		37.79[a]	ethylbenzene-d10 RT 41.97; 4-heptanone RT 42.73	MS - not available (MS found by AVM - poor fit); RT - too long
U-105	2549-67-9	Aziridine, 2-ethyl-	S5011-A14.846		35.82[a]	ethylbenzene-d10 RT 40.45; pyrazine RT 31.62	MS - not available (MS found by AVM - poor fit); RT - too long

Table 3. Misidentified Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Reference Retention Time Comparison	Comments
U-105	2549-67-9	Aziridine, 2-ethyl-	S5011-A18.385		36.22[(a)]	ethylbenzene-d10 RT 40.47; pyrazine RT 31.57	MS - not available (MS found by AVM - poor fit); RT - too long
U-105	2549-67-9	Aziridine, 2-ethyl-	S5011-A16.590		35.98[(a)]	ethylbenzene-d10 RT 40.43; pyrazine RT 31.48	MS - not available (MS found by AVM - poor fit); RT - too long
C-101	78-76-2	Butane, 2-bromo-	S4056-A13.393		38.15[(b)]	ethylbenzene-d10 RT 36.42; octane RT 31.93	MS - no reason to call it this, only 2 peaks >20% (several other earlier peaks had this compound as top computer choice); RT - too long
C-107	78-76-2	Butane, 2-bromo-	S4058-A15.701		38.42[(b)]	d5-bromobenzene RT 41.51; ethylbenzene-d10 RT 36.21; octane RT 31.76	MS - no reason to call it this, only 2 peaks >20% (several other earlier peaks had this compound as top computer choice); RT - too long
C-103	96-41-3	Cyclopentanol	S4025-D09.290		35.97[(b)]	toluene-d8 RT 30.95; octane RT 33.76	MS - poor match, no m/e 44; RT?
C-103	96-41-3	Cyclopentanol	S4025-D11.366		36.91[(b)]	toluene-d8 RT 30.94; octane RT 33.75	MS - poor match, no m/e 44; RT?
C-103	96-41-3	Cyclopentanol	S4025-D10.364	1	36.97[(b)]	toluene-d8 RT 31.01; octane RT 33.82	MS - mixture, possible, hard to tell since only 2 peaks >20% in spectrum; RT?; doesn't meet HASQARD criteria
BY-107	UAD010-01	Decadienal	S4077-A16.625		44.19[(b)]	d5-bromobenzene RT 41.63; decane 45.83	MS - poor match, no m/e 152; RT - too short
BY-107	UAD010-01	Decadienal	S4077-A17.785		42.07[(b)]	d5-bromobenzene RT 39.72; decane 43.60	MS - poor match, no m/e 152; RT - too short
BY-107	UAD010-01	Decadienal	S4077-A18.632		44.16[(b)]	d5-bromobenzene RT 41.62; decane 45.80	MS - didn't scan far enough to see m/e 152, but not likely; RT - too short
C-103	1838-59-1	Formic acid, 2-propenyl ester	S4025-D02.285		32.25[(c)]	d10-ethylbenzene RT 33.59; octane RT 29.10	MS - not very good fit, no 47, 59; RT - too long?; C7-alkene more likely
BY-105	1708-29-8	Furan, 2,5-dihydro-	S4020-A11.260		13.72[(b)]	hexafluorobenzene RT 17.54; hexane RT 16.12	MS- 41/42 ratio is wrong; Note that peak at RT 21.18 is identified as 2-butenal; RT?

Table 3. Misidentified Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Reference Retention Time Comparison	Comments
BY-105	1708-29-8	Furan, 2,5-dihydro-	S4020-A10.258		13.72[(b)]	hexafluorobenzene RT 17.59; hexane RT 16.13	MS- 41/42 ratio is wrong; Note that peak at RT 21.11 is identified as 2-butenal; RT?
BY-105	1708-29-8	Furan, 2,5-dihydro-	S4020-A13.282		13.60[(b)]	hexafluorobenzene RT 17.43; hexane RT 15.97	MS- 41/42 ratio is wrong; Note that peak at RT 21.25 is identified as 2-butenal; RT?
BY-105	1708-29-8	Furan, 2,5-dihydro-	S4020-A12.281		13.58[(b)]	hexafluorobenzene RT 17.42; hexane RT 15.97	MS- 41/42 ratio is wrong; Note that peak at RT 21.13 is identified as 2-butenal; RT?
BY-107	1708-29-8	Furan, 2,5-dihydro-	S4077-A16.625		29.93[(a)]	toluene-d8 RT 29.07; heptane RT 23.71; tetrahydrofuran RT 17.47	MS - 41/42 ratio is wrong, ; RT - too long
U-112	1708-29-8	Furan, 2,5-dihydro-	S6119-t39.309		38.81[(a)]	dodecane 42.8; benzene 16.7	RT - too long; MS - poor fit, didn't scan far enough
BY-108	3777-71-7	Furan, 2-heptyl-	S4076-A10.649	1	44.23[(b)]	d5-bromobenzene RT 41.69; decane RT 45.87	MS - not especially good fit, only 2 peaks in the spectrum are over 20%, so not enough spectral info to tell; RT ok?; doesn't meet HASQARD criteria
BY-108	3777-71-7	Furan, 2-heptyl-	S4076-A14.855	1	44.22[(b)]	d5-bromobenzene RT 41.68; decane RT 45.85	MS - not especially good fit, only 2 peaks in the spectrum are over 20%, so not enough spectral info to tell; RT ok?; doesn't meet HASQARD criteria
BY-106	4179-38-8	Furan, 2-octyl-	S4021-A11.293	1,2	66.95[(b)]	tetradecene- RT66.42; d26-dodecane RT 58.30	MS - mixture, not likely, but hard to rule out; RT - possible; more likely a branched alkene or alkyne; doesn't meet HASQARD criteria
BY-106	4179-38-8	Furan, 2-octyl-	S4021-A10.288	1,2	67.00[(b)]	tetradecene- RT66.37; d26-dodecane RT 58.27	MS - mixture, not likely, but hard to rule out; RT - possible; more likely a branched alkene or alkyne; doesn't meet HASQARD criteria

Table 3. Misidentified Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Reference Retention Time Comparison	Comments
BY-106	4179-38-8	Furan, 2-octyl-	S4021-A12.300	1,2	66.95[(b)]	tetradecene- RT66.41; d26-dodecane RT 58.30	MS - mixture, not likely, but hard to rule out; RT - possible; more likely a branched alkene or alkyne; doesn't meet HASQARD criteria
BY-106	4179-38-8	Furan, 2-octyl-	S4021-A13.304	1,2	66.96[(b)]	tetradecene- RT66.39; d26-dodecane RT 58.26	MS - mixture, not likely, but hard to rule out; RT - possible; more likely a branched alkene or alkyne; doesn't meet HASQARD criteria
BY-106	4229-91-8	Furan, 2-propyl-	S4021-A11.293	1,2	23.01[(b)]	d6-benzene RT 21.63; 2-methylhexane RT 22.23	MS-possible, but not great fit, hard to rule out, more likely a branched alkene or alkane; doesn't meet HASQARD criteria
BY-106	4229-91-8	Furan, 2-propyl-	S4021-A10.288	1,2	23.10[(b)]	d6-benzene RT 21.72; 2-methylhexane RT 22.32	MS-possible, but not great fit, hard to rule out, more likely a branched alkene or alkane; doesn't meet HASQARD criteria
BY-106	4229-91-8	Furan, 2-propyl-	S4021-A12.300	1,2	22.99[(b)]	d6-benzene RT 21.58; 2-methylhexane RT 22.20	MS-possible, but not great fit, hard to rule out, more likely a branched alkene or alkane; doesn't meet HASQARD criteria
BY-106	4229-91-8	Furan, 2-propyl-	S4021-A13.304	1,2	23.13[(b)]	d6-benzene RT 21.73; 2-methylhexane RT 22.35	MS-possible, but not great fit, hard to rule out, more likely a branched alkene or alkane; doesn't meet HASQARD criteria
BY-109	4229-91-8	Furan, 2-propyl-	S4071-610	1,2	22.01[(b)]	d6-benzene RT 20.58; 2-methylhexane RT 21.22	MS-possible, but not great fit, hard to rule out, more likely a branched alkene or alkane; doesn't meet HASQARD criteria
BY-109	4229-91-8	Furan, 2-propyl-	S4071-252	1,2	22.03[(b)]	d6-benzene RT 20.63; 2-methylhexane RT 21.27	MS-possible, but not great fit, hard to rule out, more likely a branched alkene or alkane; doesn't meet HASQARD criteria
BY-105	34314-82-4	Furan, 3-(1,1-dimethylethyl)-2,3-dihydro-	S4020-A10.258		54.00[(b)]	d26-dodecane RT 58.22; undecane RT 53.56	MS - poor fit, no m/e 93, 83; RT - too long

Table 3. Misidentified Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Notes	Retention Time	Reference Retention Time Comparison	Comments
BY-105	34314-82-4	Furan, 3-(1,1-dimethylethyl)-2,3-dihydro-	S4020-A11.260		53.99[(b)]	d26-dodecane RT 58.23; undecane RT 53.55	MS - poor fit, no m/e 93; RT - too long
BY-105	34314-82-4	Furan, 3-(1,1-dimethylethyl)-2,3-dihydro-	S4020-A13.282		54.05[(b)]	d26-dodecane RT 58.28; undecane RT 53.62	MS - poor fit, no m/e 93, 83; RT - too long
BY-105	34314-82-4	Furan, 3-(1,1-dimethylethyl)-2,3-dihydro-	S4020-A12.281		54.04[(b)]	d26-dodecane RT 58.28; undecane RT 53.60	MS - poor fit, no m/e 93, 83; RT - too long
BY-107	22431-09-0	Methanamine, N-(1-methylbutylidene)-	S4077-A16.625		32.88[(b)]	d8-toluene RT 29.07; octane RT 31.89	MS - poor match, no m/e 71, 84; RT - too long?
BY-107	22431-09-0	Methanamine, N-(1-methylbutylidene)-	S4077-A17.785		31.1[(b)]	d8-toluene RT 28.34; octane RT 30.85	MS - poor match, no m/e 71, 84; RT - too long?
BX-104	56052-94-9	Oxirane, 2-ethyl-3-propyl-, cis-	S4089-A10.565		52.77[(a)]	d26-dodecane RT 59.58; 2-nonanone RT 55.04	MS - poor match, no m/e 72, other ratios poor; RT - too long?
BX-104	56052-94-9	Oxirane, 2-ethyl-3-propyl-, cis-	S4089-A11.563		52.77[(a)]	d26-dodecane RT 59.58; 6-methylundecane RT 58.16	MS - poor match, no m/e 72, other ratios poor; RT - too long?
BX-104	56052-94-9	Oxirane, 2-ethyl-3-propyl-, cis-	S4089-A12.561		52.79[(a)]	d26-dodecane RT 59.60; 6-methylundecane RT 58.18	MS - poor match, no m/e 72, other ratios poor; RT - too long?
C-110	1795-48-8	Propane, 2-isocyanato-	S4059-A15.390		30.98[(b)]	toluene 30.10	MS - poor fit, no m/e 85, 56
U-106	694-05-3	Pyridine, 1,2,3,6-tetrahydro-	S5012-A14.829		29.53[(a)]	benzene-d6 RT 25.61; pyrazine 32.02	MS - poor fit, no m/e 68, ratios wrong

1 Failed confirmation because of HASQARD criteria.

2 Better mass spectral fit observed for alternative analyte, but still not good enough match.

(a) Gas chromatograph column conditions not available.

(b) Gas chromatograph held at 10 °C for 10 minutes, ramped to 230 °C at 3 °C per minute, held at 230 °C for 16.7 min.

(c) Gas chromatograph held at 10 °C for 5 minutes, ramped to 230 °C at 3 °C per minute, held at 230 °C for 16.7 min.

Table 4. Unreviewed Analytes

Tank	Chemical Id	Analyte Name	Field Sample Id	Comments
C-204	624-43-1	1,2,3-Propanetriol, 1-nitrate	S6067-A06.184	data package not found
C-204	3457-90-7	1,3-Propanediol, dinitrate	S6067-A04.136	data package not found
C-204	36653-82-4	1-Hexadecanol	S6067-A06.184	data package not found
C-204	112-92-5	1-Octadecanol	S6067-A04.136	data package not found
B-103	1115-11-3	2-Butenal, 2-methyl-	S6114-t45.1038	analyte not found in data package
C-204	4176-04-9	Bicyclo[4.1.0]heptan-3-one, 4,7,7-trimethyl-, [1R- (1.alpha.,4.alpha.,6.alpha.)]-	S6067-A04.136	data package not found
C-204	627-05-4	Butane, 1-nitro-	S6067-A04.136	data package not found
C-204	627-05-4	Butane, 1-nitro-	S6067-A05.153	data package not found
C-204	627-05-4	Butane, 1-nitro-	S6067-A06.184	data package not found
C-204	627-05-4	Butane, 1-nitro-	S6067-A12.1078	data package not found
C-204	627-05-4	Butane, 1-nitro-	S6067-A13.1079	data package not found
C-204	627-05-4	Butane, 1-nitro-	S6067-A11.1077	data package not found
C-204	89-82-7	Cyclohexanone, 5-methyl-2-(1-methylethylidene)-, (R)-	S6067-A06.184	data package not found
AX-103	3777-69-3M	Furan, 2-pentyl- and others	S5029-A16.993	data package not found

Appendix A

HASQARD Guidelines

6.7.7 Tentatively Identified Compounds

A project/program may specify criteria for determination of tentatively identified compounds (TIC). The following criteria are suggested for consideration when making a project/program specification or may be used in lieu of such specifications.

The library match for a TIC should be higher than 75% before this detailed evaluation is initiated. The method-specified tune criteria should be met. Special attention to the tune at low masses should be taken when evaluating volatile compounds. The concentration of a TIC should be greater than 10% of the nearest internal standard or estimated 5 nanogram on column injection, whichever is smaller. Early (injection peak) and late eluting peaks (column bleed and coeluting compounds) should have adequate background subtraction to permit use of these TIC criteria. If isotopic patterns are present, the mass ratios should agree with the reference spectrum within 10%. The base mass peak for the sample should be the same as the reference spectrum. If a molecular ion is present in the reference spectrum, the sample should also have a molecular ion mass. Reference spectrum ions greater than 20% should be in the sample spectrum. Sample ions greater than 20% that are not in the reference spectrum need to be evaluated. Major sample ions (greater than 20%) should match relative intensities to the base peak to those same ratios for the reference spectrum within 10-30%.

If a peak is determined to not meet the criteria for a TIC, the criteria for which it failed should be documented, so that it will not have to be evaluated again in the future.

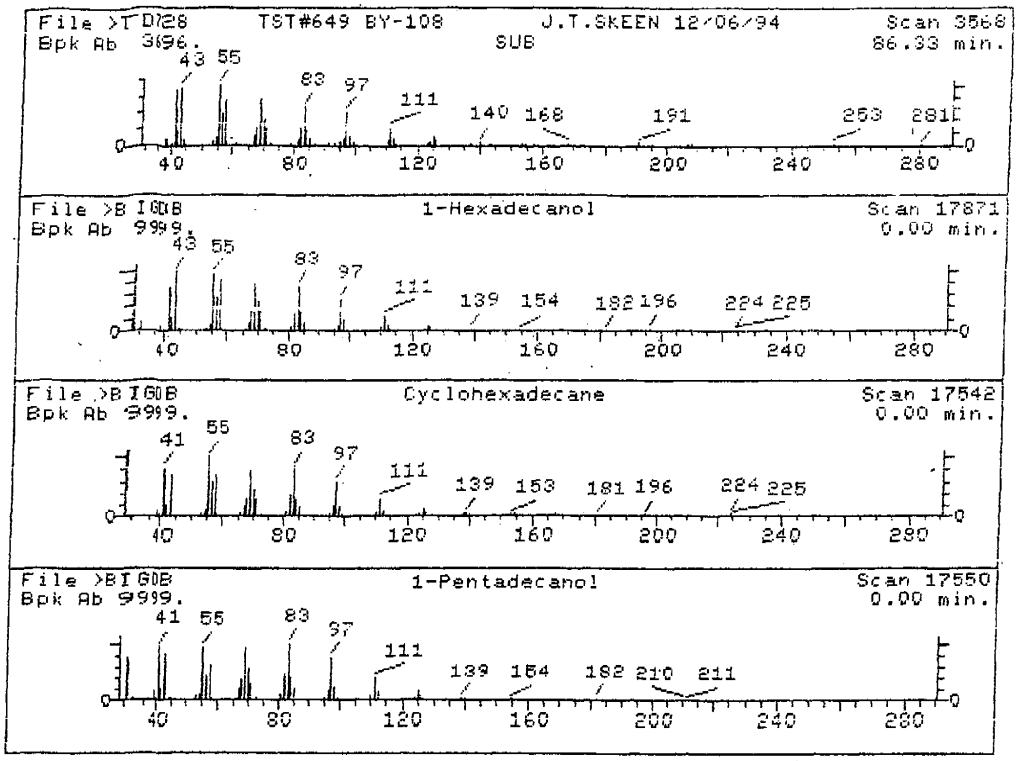
A TIC compound may be upgraded to a positively identified compound (PIC). This is achieved by obtaining the compound, analyzing it under same conditions as the initial identification, and matching retention time and mass spectrum. This may be done at the customer's request if they deem it necessary for the program.

It is highly recommended that only PICs be added to target analyte lists.

Appendix B

Spectra Data

Table 1. Confirmed Analyses



. UNKNOWN #.,176,. OF .,181

①	1-Hexadecanol	242 C16H34O
2.	Cyclohexadecane	224 C16H32
3.	1-Pentadecanol	228 C15H32O
4.	1-Octadecanol	270 C18H38O
5.	16-METHYLHEPTADECANOL-1	270 C18H38O

Sample file: >TD728 Spectrum #: 3568
Search speed: 1 Tilting option: N No. of ion ranges searched: 49

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	93	36653824	17871	"BIGDB	147	14	2	0	75	0	68	80
2.	89	295658	17542	"BIGDB	134	22	2	0	75	0	66	67
3.	89	629765	17550	"BIGDB	132	31	2	0	62	0	66	67
4.	88	112925	17632	"BIGDB	129	41	3	0	70	0	65	56
5.	88	0	17631	"BIGDB	127	42	3	0	69	0	65	53

Data File: /chem/hpdos4.i/46112601.b/46112605.d

Date : 26-NOV-1996 14:27

Client ID : S6114-m28.1027

Instrument: hpdos4.i

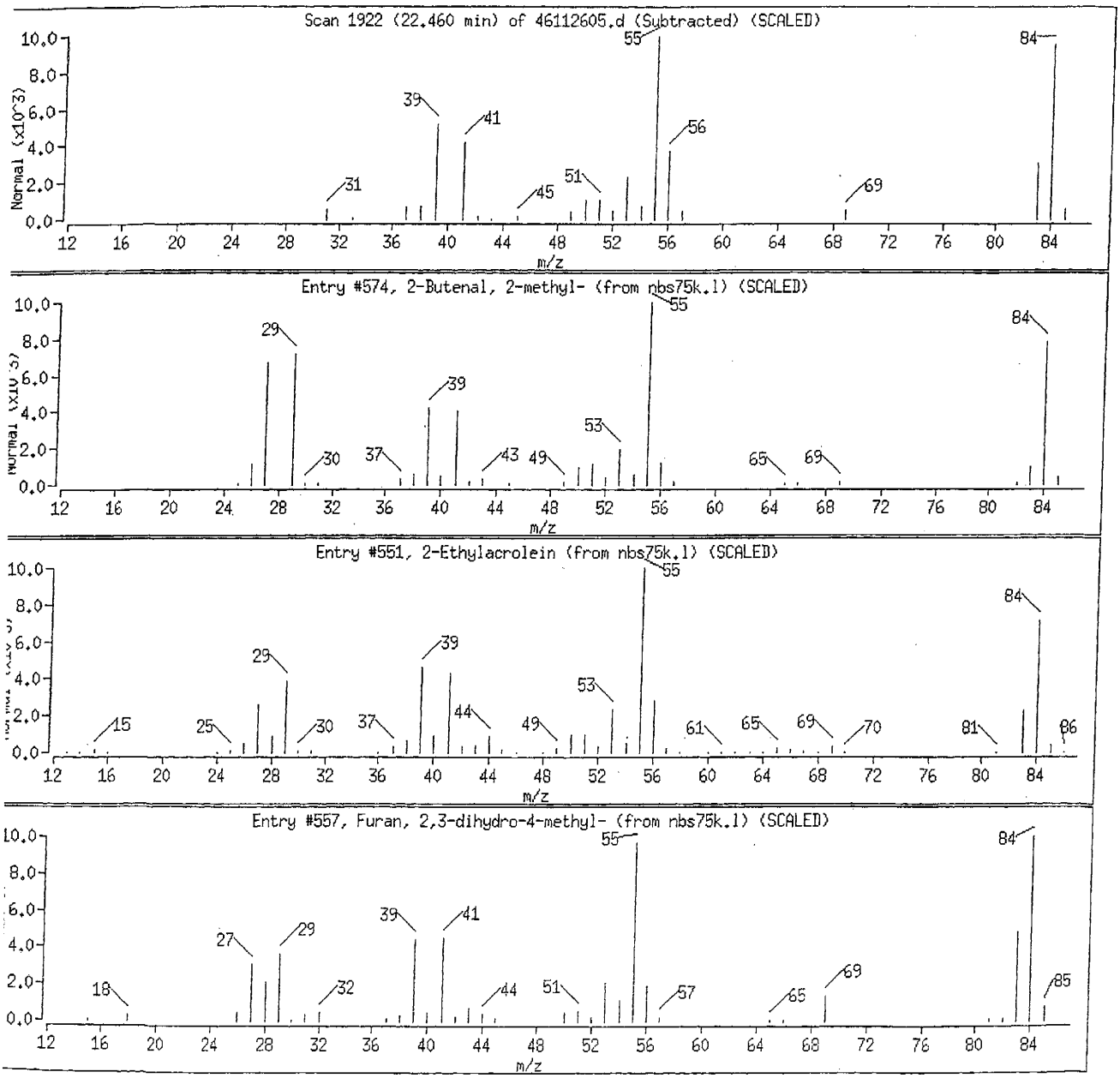
Sample Info: B-103 S6114-m28.1027

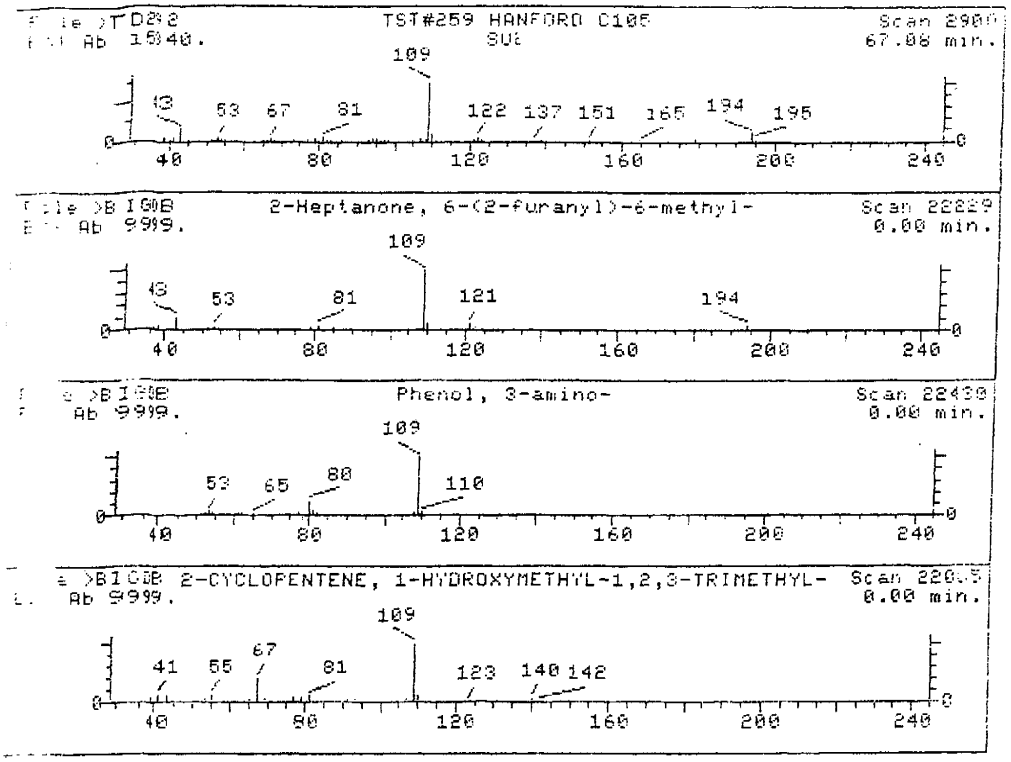
Operator: JLJ

Column phase: DB-1

Column diameter: 0.32

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butenal, 2-methyl-	1115-11-3	nbs75k.l	574	90	C5H8O	84
2-Ethylacrolein	922-63-4	nbs75k.l	551	87	C5H8O	84
Furan, 2,3-dihydro-4-methyl-	34314-83-5	nbs75k.l	557	78	C5H8O	84





0.140 %

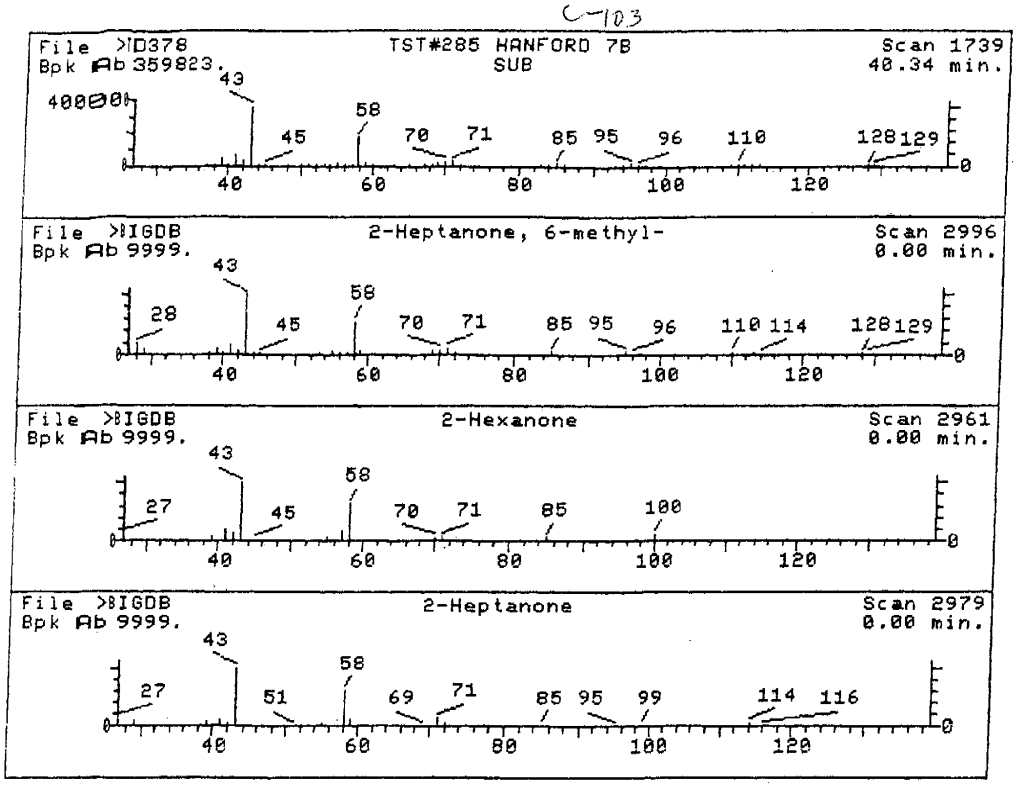
UNKNOWN #.,100,. OF .,14n

.	2-Heptanone, 6-(2-furanyl)-6-methyl-	194 C12H ·02
.	Phenol, 3-amino-	109 C6H7NO
.	2-CYCLOPENTENE, 1-HYDROXYMETHYL-1,2,3-TRIMETHYL-	140 C9Hi6O
.	Pyridine, 4-methoxy-	109 C6H7NO
.	2H-Pyrrol-2-one, 1,5-dihydro-5-methoxy-3,5-dimethyl-	141 C7Hi J2

: mple file: >TD292 Spectrum #: 2900
-arch speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#F	TIL	%	CO	C_	R_IV
..	52*	51995870	22229	"BIGDB	26	36	1	0	100	20	20	14
	45*	591275	22430	"BIGDB	40	30	1	0				
	45	0	22085	"B -DB	45	42		0			1	16
	43*	620086	22327				2	0	100			1
		591		86	"B -DB			2	0	100		1	14

C-103



45.25

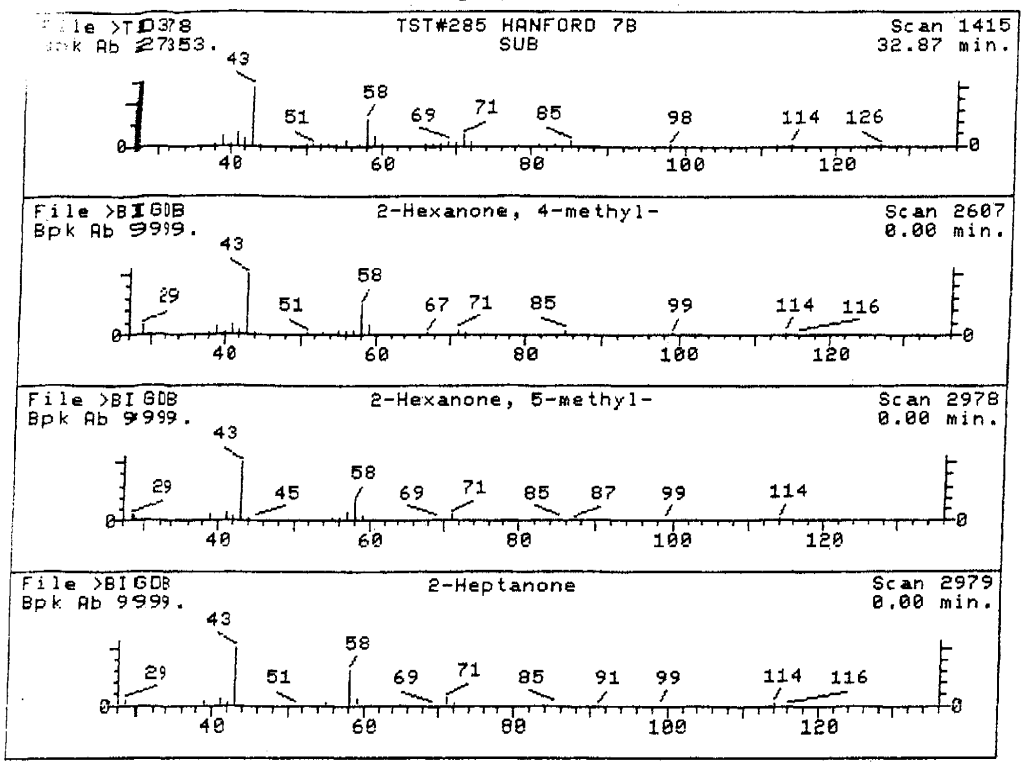
UNKNOWN #.,66,. OF .,100

1.	2-Heptanone, 6-methyl-	128 C8H16O
2.	2-Hexanone	100 C6H12O
3.	2-Heptanone	114 C7H14O
4.	2-Heptanone	114 C7H14O
5.	2-Propanone	58 C3H6O

Sample file: >TD378 Spectrum #: 1739
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_I
1.	61*	928687	2996	"BIGDB	47	27	0	0	44	44	18	6
	60	591786	2961	"BIGDB	40	43	2	0	76	15	30	1
	60	110430	2979	"BIGDB	36	47	2	0	81	15	30	1
	60	110430	2605	"BIGDB	35	48	2	0	89	15	30	1
	52*	67641	2894	"BIGDB	22	47	1	0	89	16	20	1

C-103



UNKNOWN #.,51,. OF .,100

1.	2-Hexanone, 4-methyl-	114 C7H14O
2.	2-Hexanone, 5-methyl-	114 C7H14O
3.	2-Heptanone	114 C7H14O
4.	2-Octanone	128 C8H16O
5.	2-Heptanone	114 C7H14O

Sample file: >TD378 Spectrum #: 1415
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	70	105420	2607	"BIGDB	41	45	2	0	89	10	42	14
2.	70	110123	2978	"BIGDB	37	43	2	0	100	10	42	12
3.	70	110430	2979	"BIGDB	38	45	2	0	75	7	42	13
4.	70	111137	2998	"BIGDB	36	46	2	0	79	6	42	12
5.	60*	110430	2981	"BIGDB	33	47	1	0	78	12	30	18

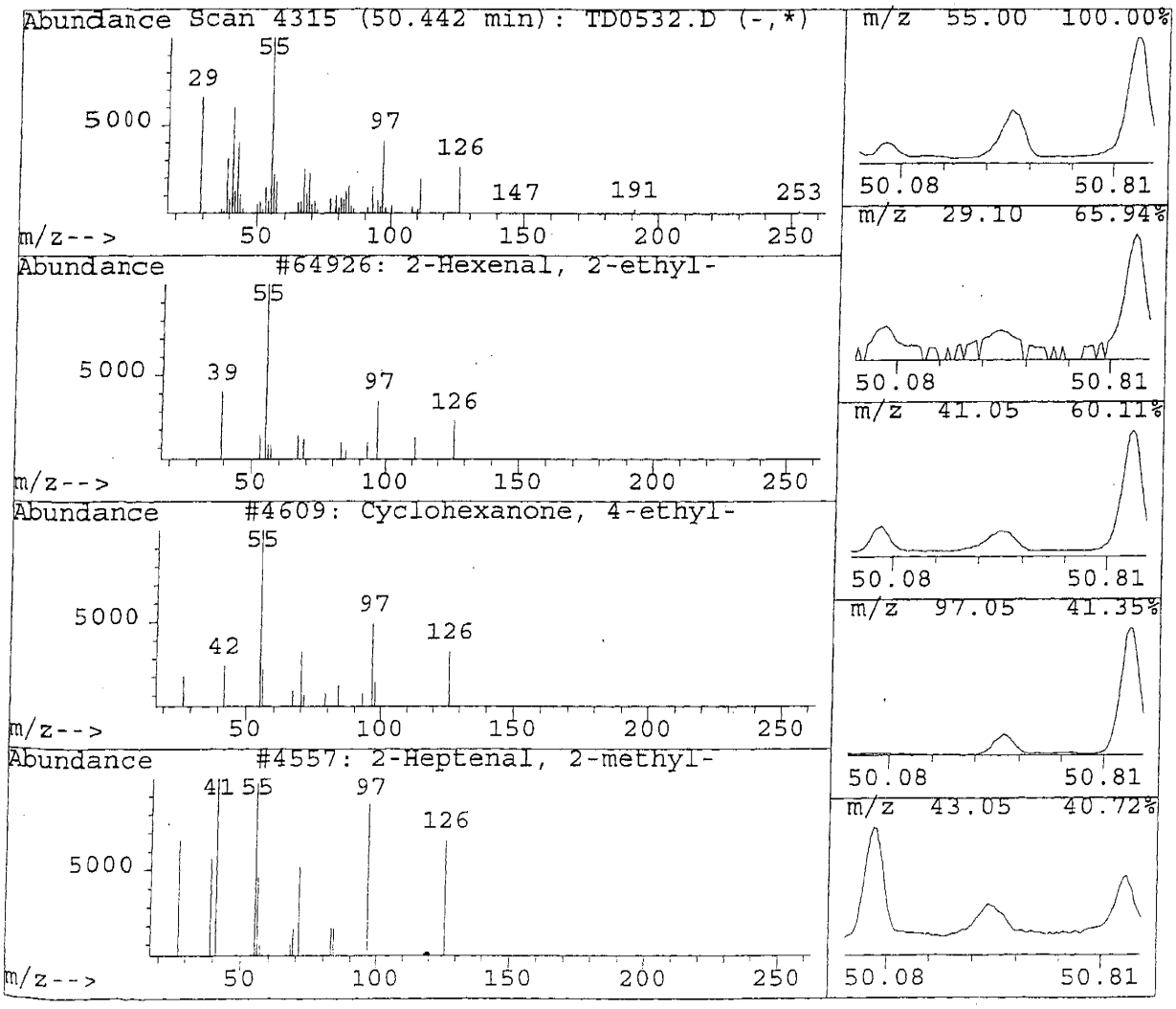
Data File : C:\HPCHEM\1\DATA\TODD\TD0532.D
Acq On : 31 Jul 95 2:28 pm
Sample : TST#1004 AX-102 1.0L
Misc : SAMPLED 6/27/95

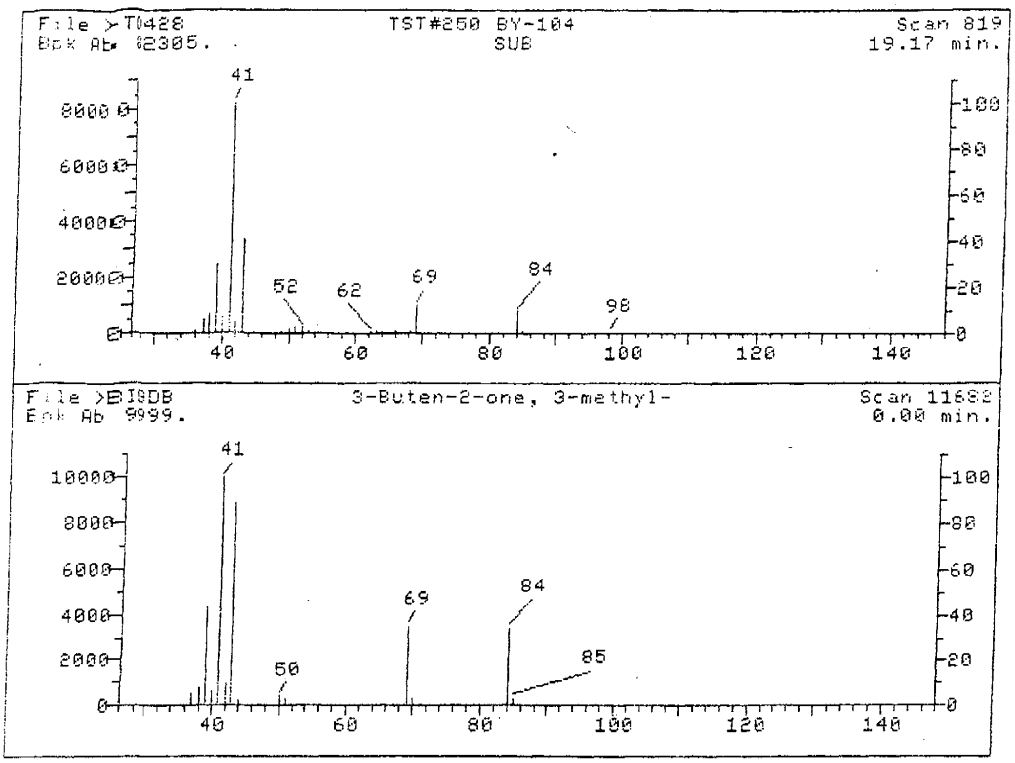
Vial: 1
Operator: J.T. SKEEN
Inst : 5972 - In
Multiplr: 1.00

Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
50.44	13.01 NG	307694	ETHYLBENZENE-D10	41.47

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	2-Hexenal, 2-ethyl-	64926	000645-62-5	72
2	Cyclohexanone, 4-ethyl-	4609	005441-51-0	68
3	2-Heptenal, 2-methyl-	4557	030567-26-1	47
4	Cyclohexane, 1,2-dimethyl- (cis/tra	2699	000583-57-3	35
5	(Z)-4-C9H18	4673	010405-84-2	35





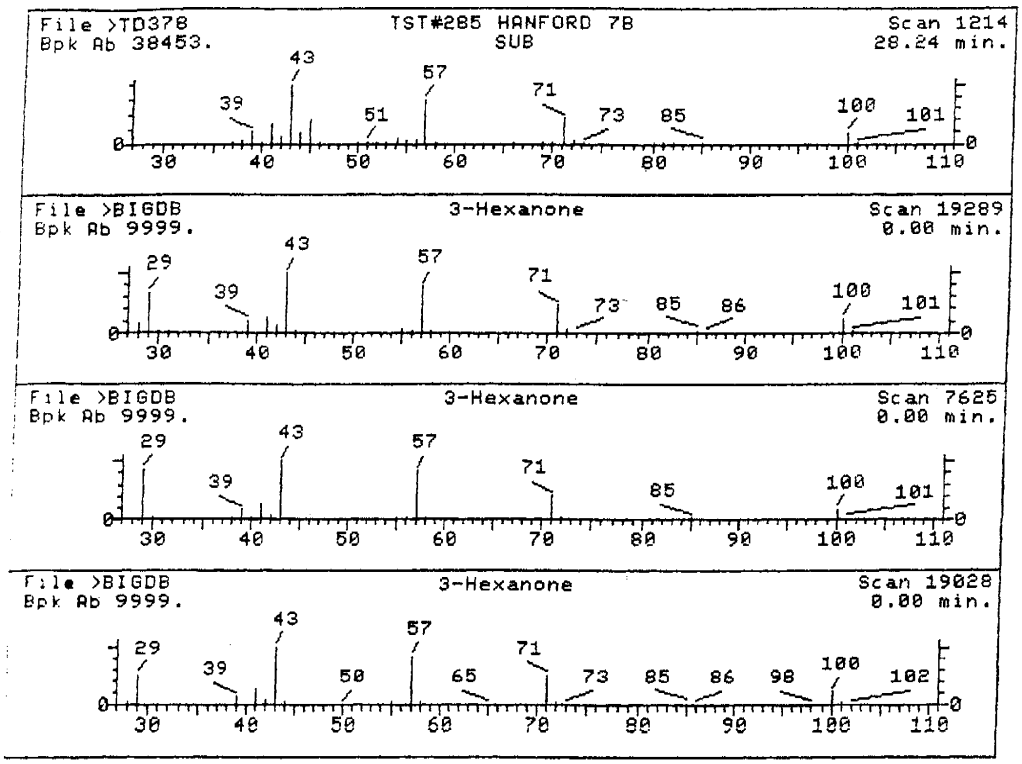
UNKNOWN #.,51,. OF .,190

1. 3-Buten-2-one, 3-methyl- 84 C5H8O

Sample file: >TD428 Spectrum #: 819
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CO	C_	R_IU
1.	12*	814788	11682	"BIGDB	29	34	0	0	31	64	2	21

C-103



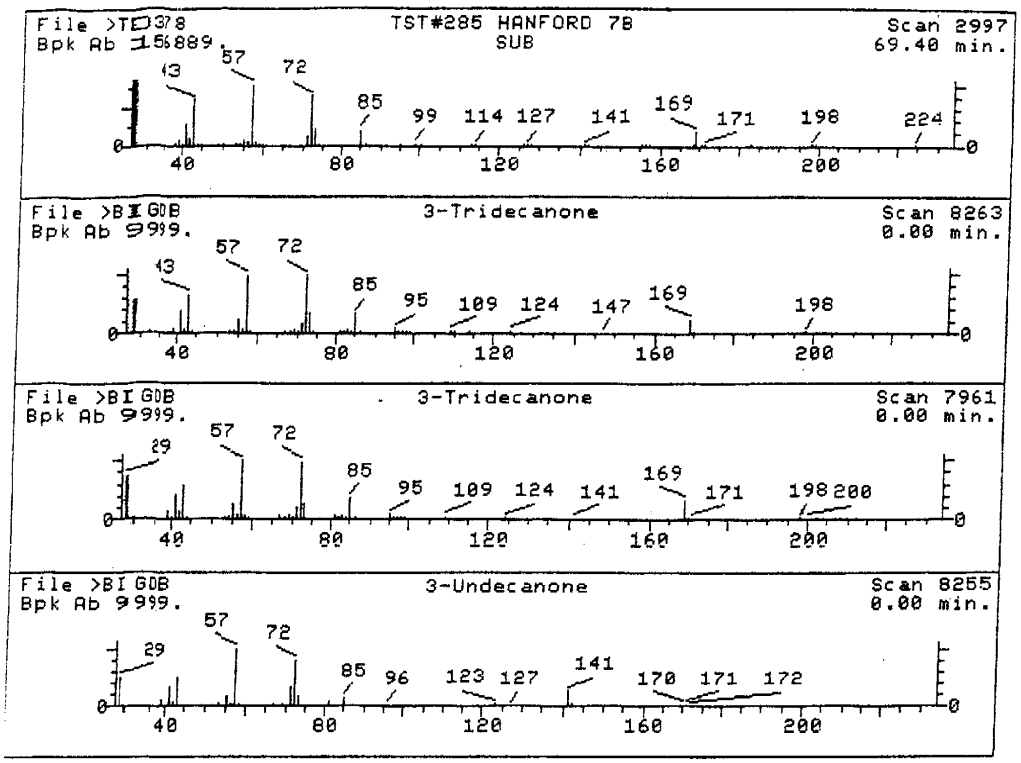
. UNKNOWN #.,41,. OF .,100

✓1.	3-Hexanone	100 C6H120
2.	3-Hexanone	100 C6H120
3.	3-Hexanone	100 C6H120
4.	3-Hexanone	100 C6H120
5.	3-Pentanone, 2-methyl-	100 C6H120

Sample file: >TD378 Spectrum #: 1214
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_I
1.	81*	589388	19289	"BIGDB	61	29	0	0	70	18	45	73
2.	70*	589388	7625	"BIGDB	46	45	0	0	71	20	32	54
3.	66*	589388	19028	"BIGDB	54	34	1	0	80	18	31	46
4.	58*	589388	19288	"BIGDB	41	49	2	0	95	18	25	21
5.	42*	565695	19283	"BIGDB	39	44	2	0	73	30	14	19

C-103



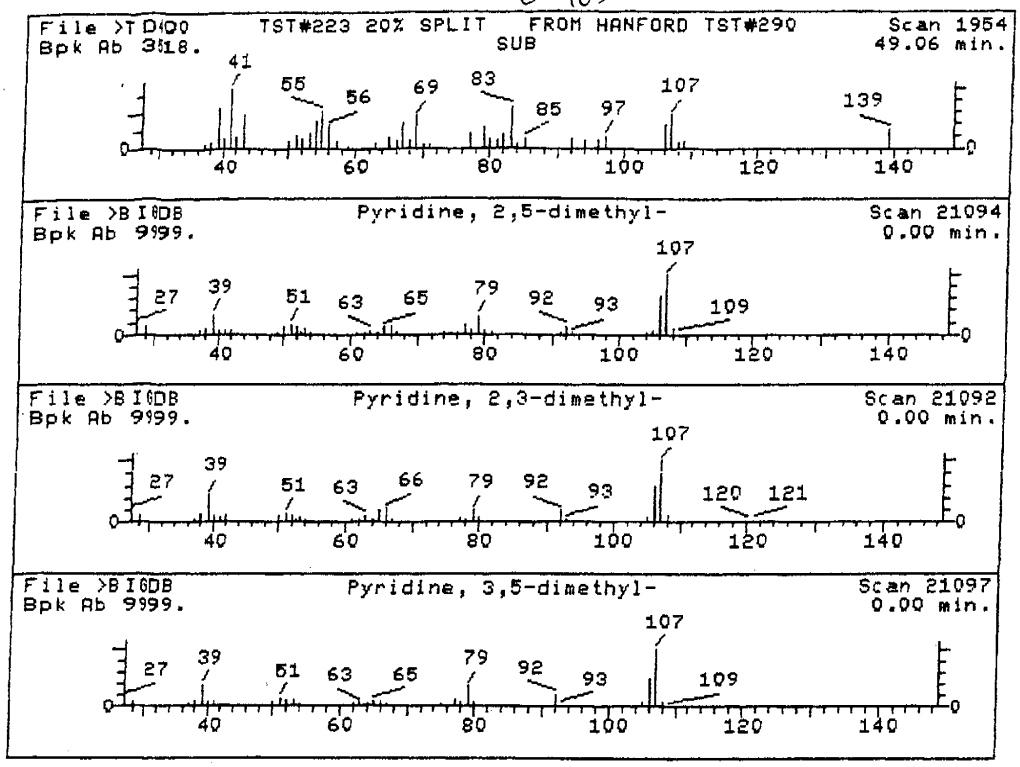
UNKNOWN #.,82,. OF .,100

1.	3-Tridecanone	198 C13H26O
2.	3-Tridecanone	198 C13H26O
3.	3-Undecanone	170 C11H22O
4.	3-Undecanone	170 C11H22O
5.	2-Propen-1-ol, 2-methyl-	72 C4H8O

Sample file: >TD378 Spectrum #: 2997
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_I
1.	78	1534265	8263	"BIGDB	67	49	2	0	74	1	55	14
2.	78	1534265	7961	"BIGDB	68	58	2	0	71	1	55	15
3.	52*	2216877	8255	"BIGDB	33	65	3	0	100	19	20	13
4.	41*	2216877	8256	"BIGDB	22	76	3	0	100	21	17	12
5.	35*	513428	8136	"BIGDB	22	96	3	0	100	29	14	12

C 103



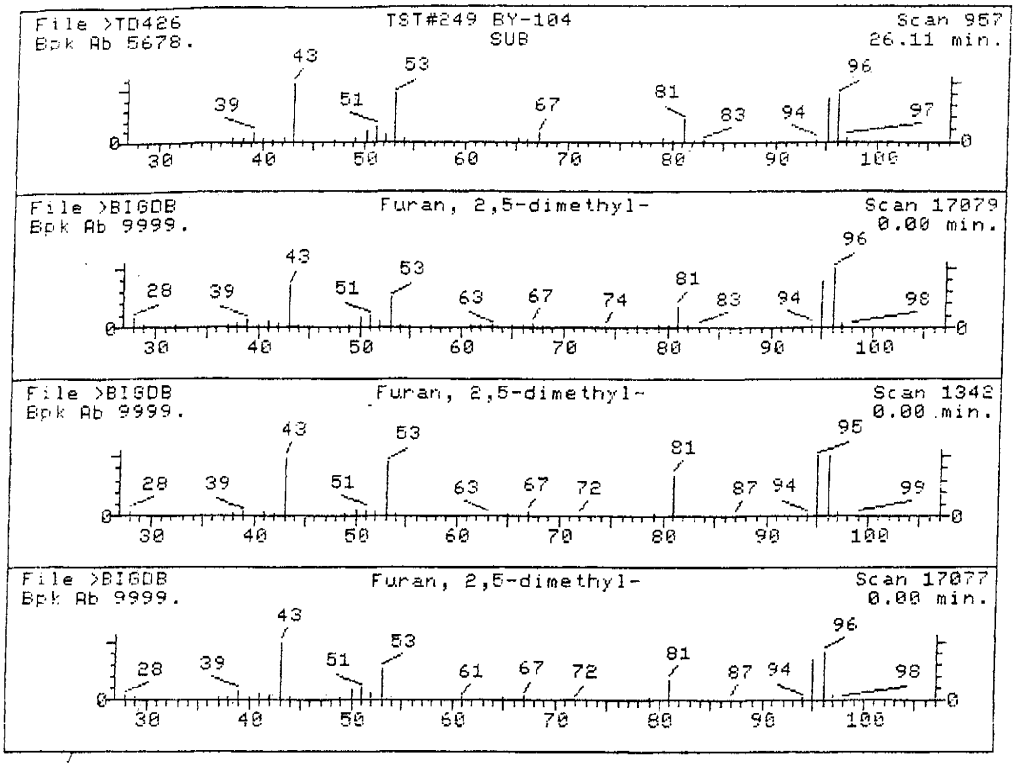
C_2-pyridine and others

. UNKNOWN #.,62,. OF .,137

1.	Pyridine, 2,5-dimethyl-	107 C7H9N
2.	Pyridine, 2,3-dimethyl-	107 C7H9N
3.	Pyridine, 3,5-dimethyl-	107 C7H9N
4.	Pyridine, 3,4-dimethyl-	107 C7H9N
5.	Pyridine, 4-ethyl-	107 C7H9N

Sample file: >TD400 Spectrum #: 1954
Search speed: 1 Tilting option: N No. of ion ranges searched: 45

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	13*	589935	21094	"BIGDB	50	58	1	0	55	61	3	32
2.	13*	583619	21092	"BIGDB	56	56	2	0	55	62	3	33
3.	12*	591220	21097	"BIGDB	45	62	1	0	55	62	2	21
4.	12*	583584	21096	"BIGDB	45	65	1	0	55	65	2	21
5.	11*	536754	21099	"BIGDB	40	57	3	0	46	64	2	13



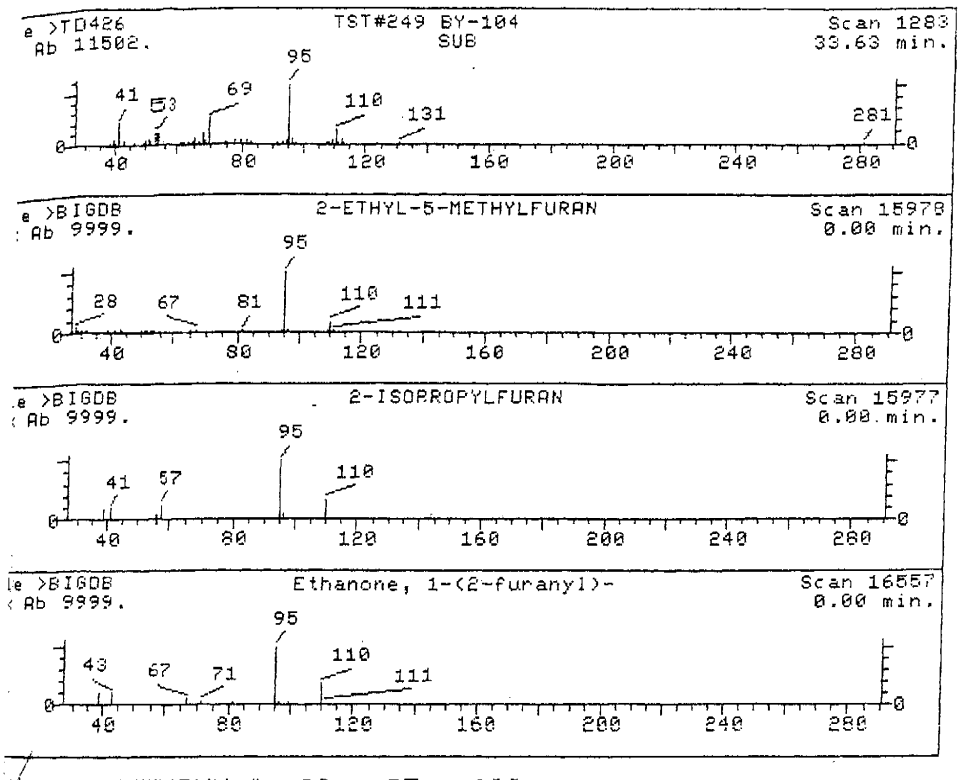
UNKNOWN #.,59,. OF .,199

1.	Furan, 2,5-dimethyl-	96 C6H8O
2.	Furan, 2,5-dimethyl-	96 C6H8O
3.	Furan, 2,5-dimethyl-	96 C6H8O
4.	Furan, 2,5-dimethyl-	96 C6H8O
5.	Furan, 2,5-dimethyl-	96 C6H8O

Sample file: >TD426 Spectrum #: 957
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CO	C_	R_I
1.	75*	625865	17079	"BIGDB	66	38	1	0	78	20	35	66
2.	71*	625865	1342	"BIGDB	54	49	2	0	71	15	38	31
3.	70*	625865	17077	"BIGDB	61	49	1	0	82	20	32	57
4.	64*	625865	17081	"BIGDB	37	36	0	0	76	24	[illegible]	[illegible]
5.	51*	625865	17078	"BIGDB	54	50	2	0	78	28	[illegible]	31

0.076



UNKNOWN #.,82,. OF .,199

1.	2-ETHYL-5-METHYLFURAN	110 C7H10O
2.	2-ISOPROPYLFURAN	110 C7H10O
3.	Ethanone, 1-(2-furanyl)-	110 C6H6O2
4.	Ethanone, 1-(2-furanyl)-	110 C6H6O2
5.	Ethanone, 1-(1H-pyrazol-4-yl)-	110 C5H6N2O

Sample file: >TD426 Spectrum #: 1283
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IN
1.	60*	0	15978	"BIGDB	32	42	1	0	100	11	30	17
2.	52*	0	15977	"BIGDB	23	24	2	0	71	19	20	13
3.	52*	1192627	16557	"BIGDB	28	31	2	0	67	19	20	14
4.	52*	1192627	16554	"BIGDB	34	45	2	0	69	17	20	17
5.	52*	25016164	15973	"BIGDB	27	54	2	0	74	17	20	14

099

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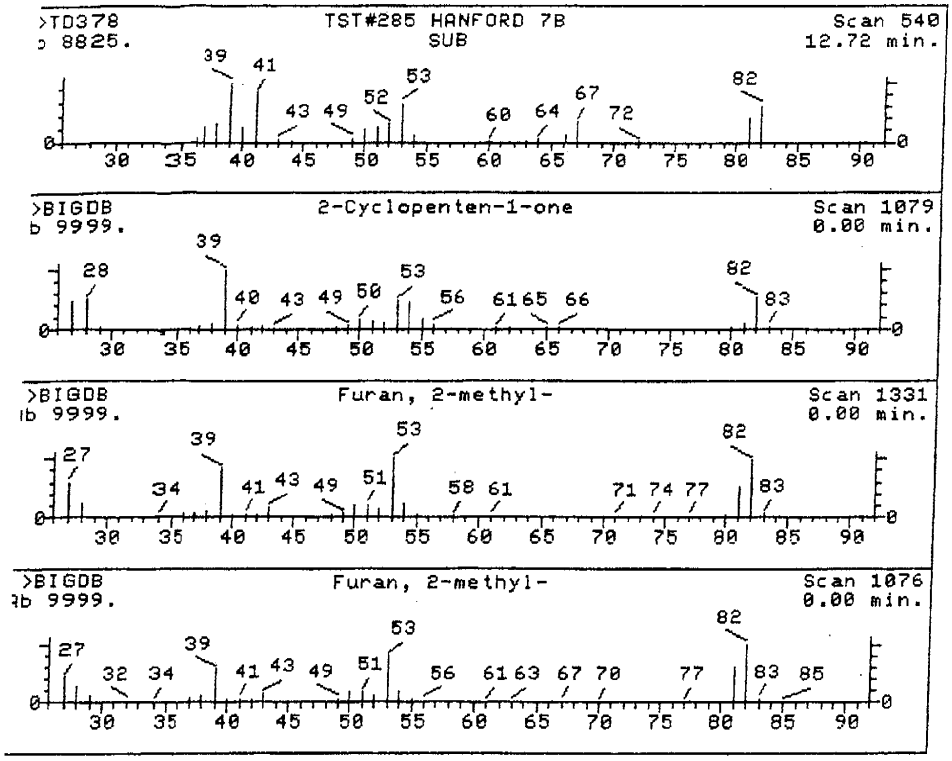


UNKNOWN #.,18,. OF .,100

.	2-Cyclopenten-1-one	82 C5H6O
.	Furan, 2-methyl-	82 C5H6O
.	Furan, 2-methyl-	82 C5H6O
.	Furan, 2-methyl-	82 C5H6O
.	2-Cyclopenten-1-one	82 C5H6O

mple file: >TD378 Spectrum #: 540
rch speed: 1 Tilting option: N No. of ion ranges searched: 40

Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
36*	930303	1079	"BIGDB	42	68	3	0	100	27	14	13
28*	534225	1331	"BIGDB	30	74	1	0	47	45	8	16
20*	534225	1076	"BIGDB	40	69	2	0	61	52	5	14
15*	534225	1332	"BIGDB	20	48	1	0	61	60	3	14
11*	930303	1333	"BIGDB	25	83	3	0	61	61	2	13

Library Search Compound Report

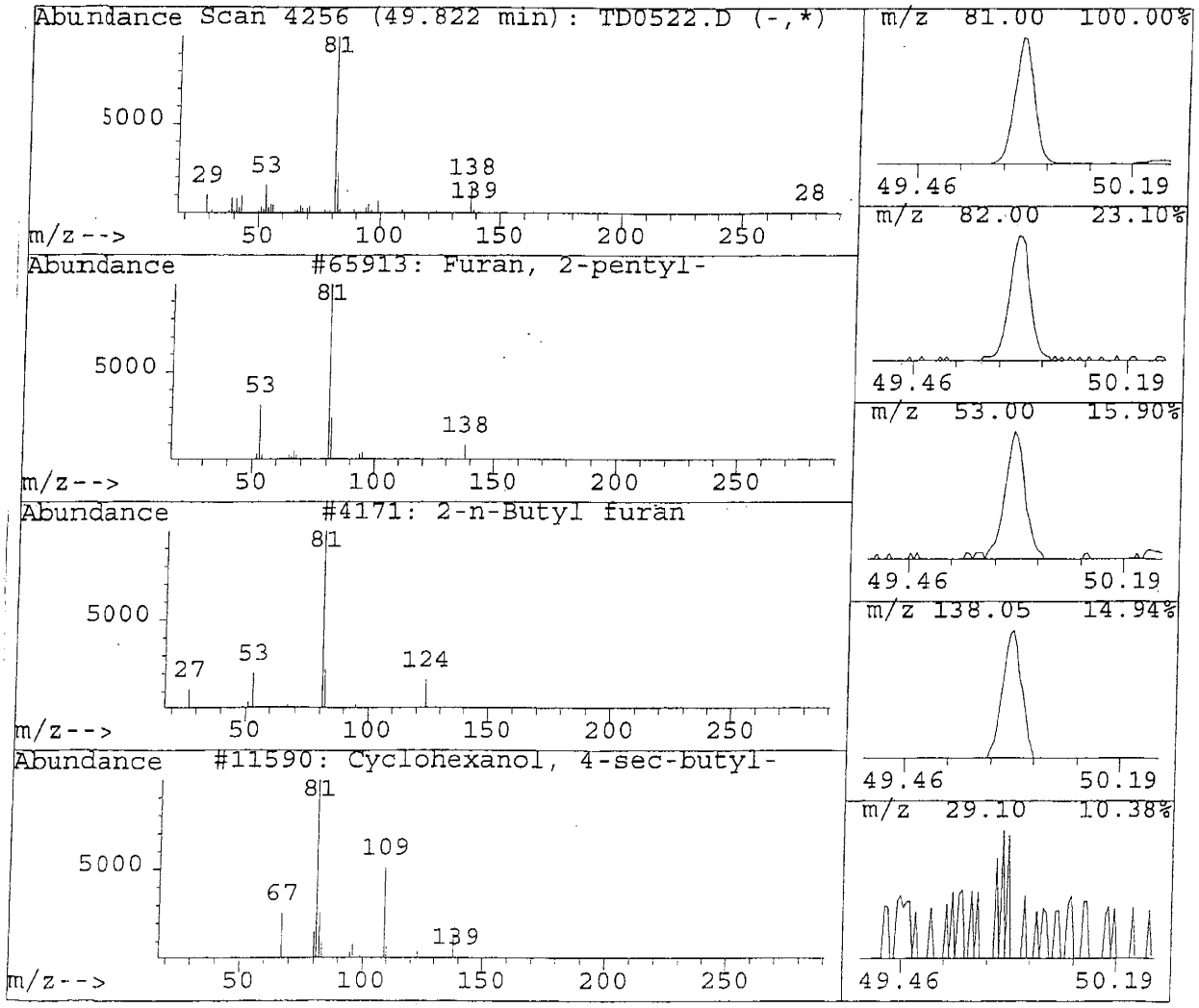
Data File : C:\HPCHEM\1\DATA\TODD\TD0522.D
Acq On : 27 Jul 95 11:38 am
Sample : TST#976 AX-101 1.0L
Misc : SAMPLED 6/15/95

Vial: 1
Operator: J.T. SKEEN
Inst : 5972 - In
Multiplr: 1.00

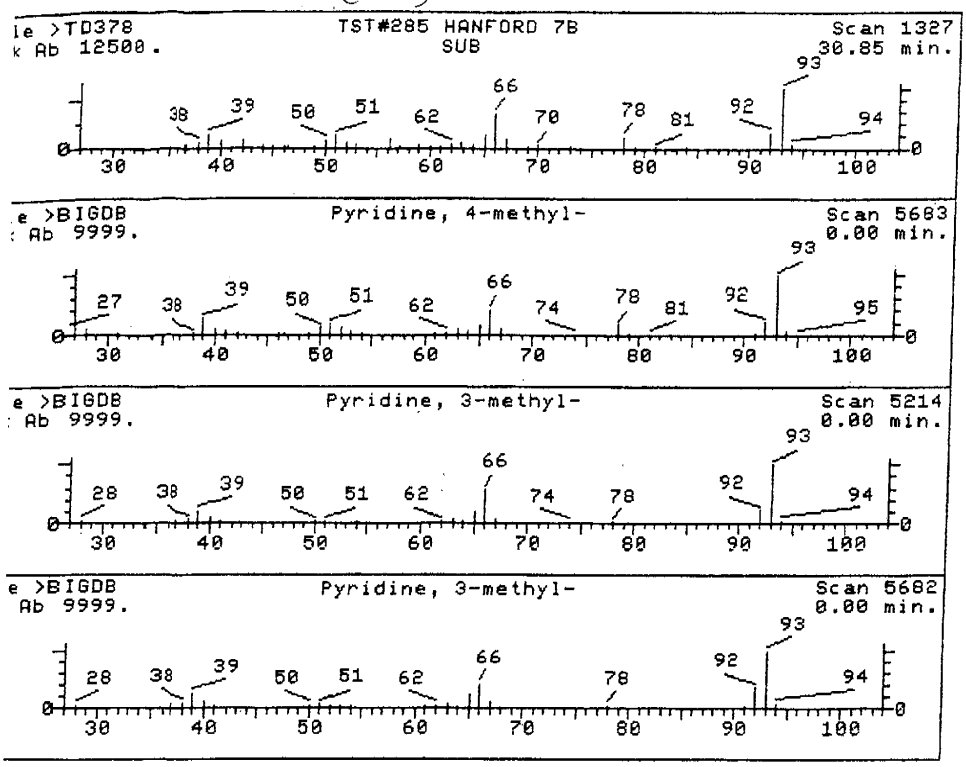
Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
49.82	14.65 NG	324663	ETHYLBENZENE-D10	41.53

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	Furan, 2-pentyl-	65913	003777-69-3	90
2	2-n-Butyl furan	4171	004466-24-4	50
3	Cyclohexanol, 4-sec-butyl-	11590	006292-20-2	40
4	2-Hexylfuran	10291	000000-00-0	38
5	2,4-Hexadienal, (E,E)-	63121	000142-83-6	36



C-103



methylpyridine

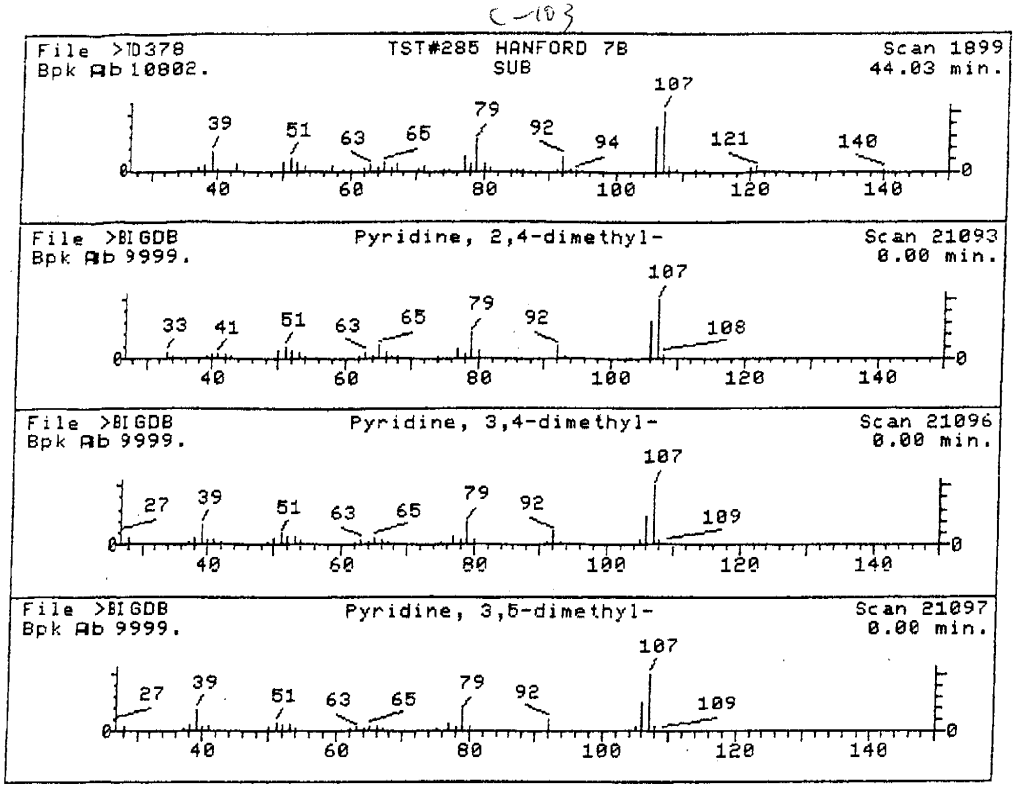
UNKNOWN #.,48,. OF .,100

1.	Pyridine, 4-methyl-	93 C6H7N
2.	Pyridine, 3-methyl-	93 C6H7N
3.	Pyridine, 3-methyl-	93 C6H7N
4.	Pyridine, 2-methyl-	93 C6H7N
5.	Pyridine, 2-methyl-	93 C6H7N

mple file: >TD378 Spectrum #: 1327
arch speed: 1 Tilting option: N No. of ion ranges searched: 41

Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
88*	108894	5683	"BIGDB	74	32	2	0	100	2	65	56
81*	108996	5214	"BIGDB	71	18	1	0	100	18	45	77
81*	108996	5682	"BIGDB	64	33	0	0	71	25	41	77
75*	109068	5675	"BIGDB	70	36	1	0	78	20	35	69
75*	109068	5678	"BIGDB	66	42	1	0	81	20	35	66

C-103

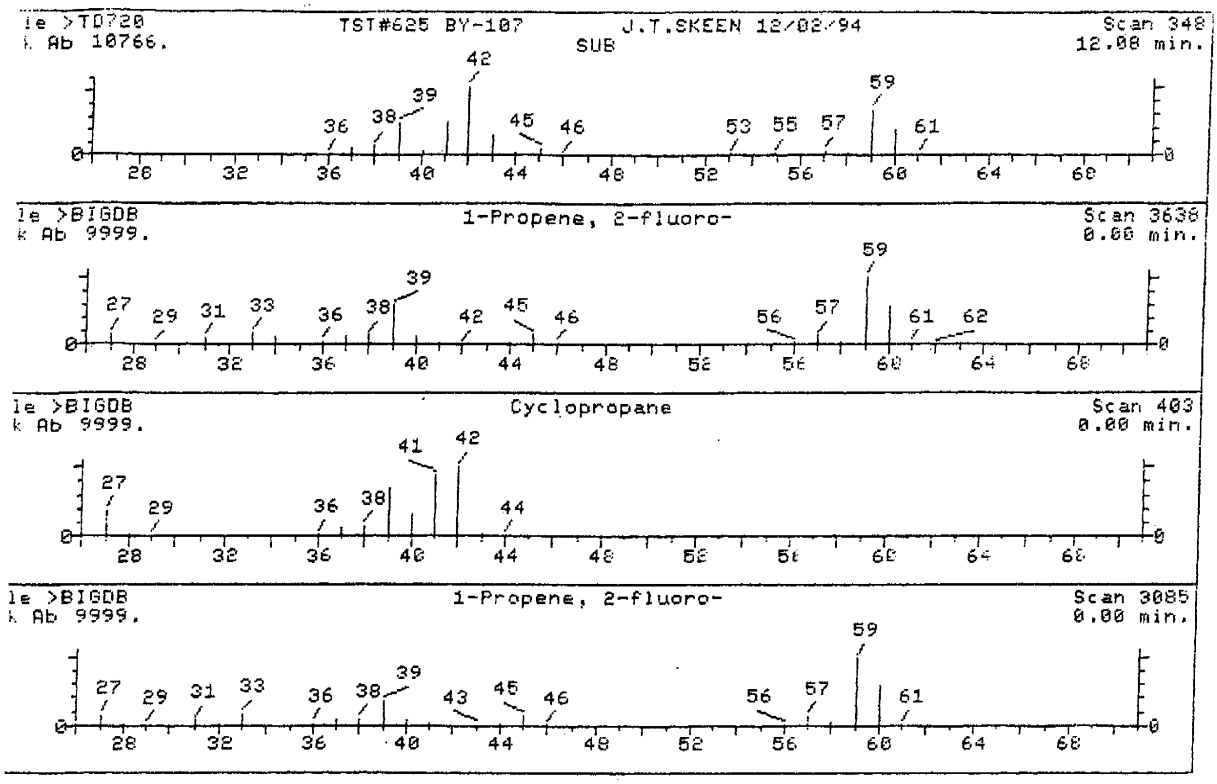


UNKNOWN #.,72,. OF .,100

1.	Pyridine, 2,4-dimethyl-	107 C7H9N
2.	Pyridine, 3,4-dimethyl-	107 C7H9N
3.	Pyridine, 3,5-dimethyl-	107 C7H9N
4.	Pyridine, 2,5-dimethyl-	107 C7H9N
5.	Pyridine, 3-ethyl-	107 C7H9N

Sample file: >TD378 Spectrum #: 1899
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	83*	108474	21093	"BIGDB	72	46	2	0	98	8	54	54
2.	76*	583584	21096	"BIGDB	72	38	2	0	100	12	40	54
3.	70*	591220	21097	"BIGDB	60	47	1	0	81	19	32	56
4.	68*	589935	21094	"BIGDB	71	37	2	0	96	25	30	52
5.	67*	536787	21514	"BIGDB	60	48	1	0	87	26	27	56

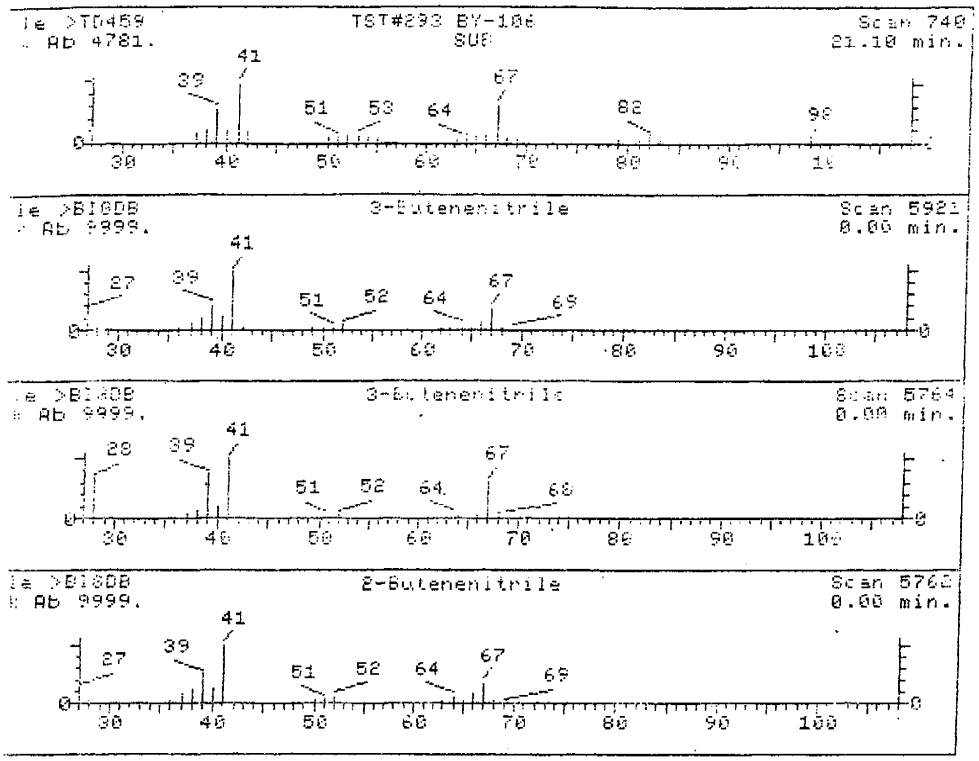


UNKNOWN #.,10,. OF .,175

(1)	1-Propene, 2-fluoro-	60 C3H5F
2.	Cyclopropane	42 C3H6
3.	1-Propene, 2-fluoro-	60 C3H5F
4.	Cyclopropane	42 C3H6
5.	1-Propene, 3-fluoro-	60 C3H5F

Sample file: >TD720 Spectrum #: 348
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROOT	K	Dk	#FLG	TILT	%	CON	C_I	R_IU
1.	42*	1184607	3638	"BIGDB	54	54	2	0	59	39	17	31
2.	31*	75194	403	"BIGDB	35	57	2	0	67	40	10	17
3.	21*	1184607	3085	"BIGDB	48	44	1	0	50	58	5	35
4.	15*	75194	402	"BIGDB	27	60	1	0	51	57	3	15
5.	15*	818928	3086	"BIGDB	23	71	2	0	67	60	3	13



UNKNOWN #.,44,. OF .,2[illegible]

1.	3-Butenenitrile	67 C4H5N
2.	3-Butenenitrile	67 C4H5N
3.	2-Butenenitrile	67 C4H5N
4.	1H-Pyrrole	67 C4H5N
5.	1H-Pyrrole	67 C4H5N

Sample file: >TD459 Spectrum #: 74[illegible]
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DF	#F	S	TIMT	%	CO	C_	R_
.	[illegible]3*	109751	5921	"B[illegible]-DB	58	39	0		0	87	28	37	71
.	73*	109751	5764	"B[illegible]GDB	51	44	0		0	78	25	3[illegible]	6[illegible]
.	[illegible]6*	4786[illegible]03	5762	"B[illegible]-DB	60	56	2		0	74	38	14	[illegible]3
.	34*	109977	5917	"B[illegible]GDB	39	6[illegible]	1		0	5[illegible]	3[illegible]	1[illegible]	2[illegible]
.	[illegible]3*	109977	5916	"B[illegible]-DB	35	58	1		0	65	36	10	19

Library Search Compound Report

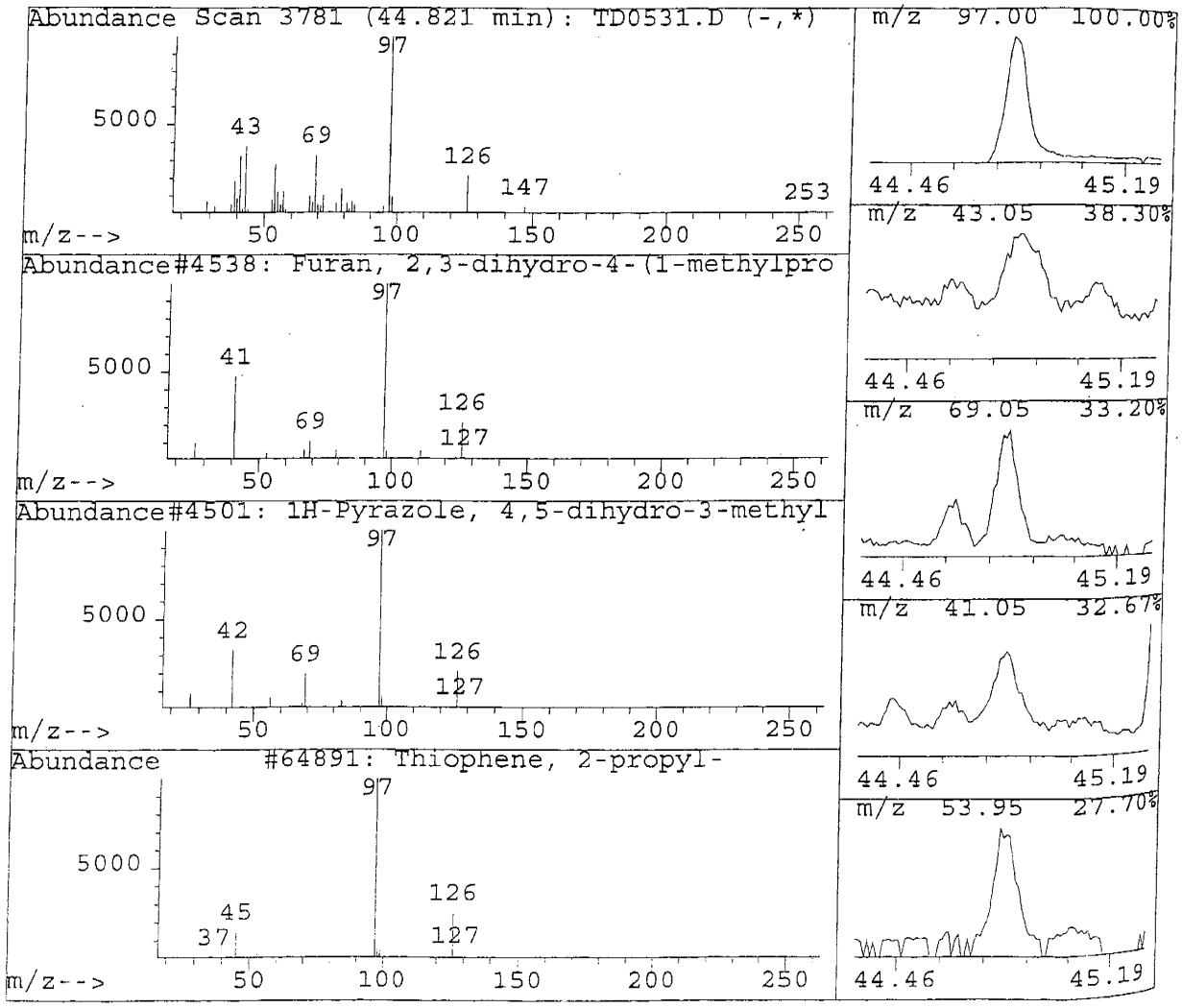
Data File : C:\HPCHEM\1\DATA\TODD\TD0531.D
Acq On : 31 Jul 95 11:56 am
Sample : TST#1003 AX-102 1.0L
Misc : SAMPLED 6/27/95

Vial: 1
Operator: J.T.
Inst : 5972
Multiplr: 1.00

Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
44.82	5.52 NG	104063	ETHYLBENZENE-D10	41.48

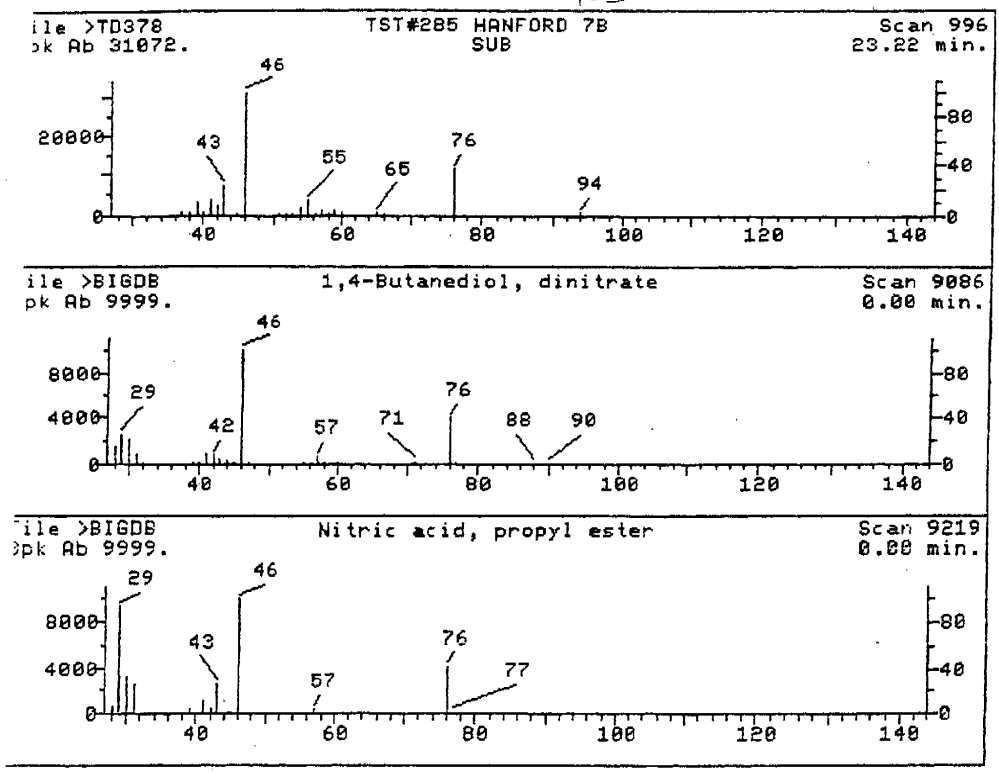
Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	Furan, 2,3-dihydro-4-(1-methylpropyl)-	4538	034379-54-9	53
2	1H-Pyrazole, 4,5-dihydro-3-methyl-1	4501	026964-49-8	50
3	Thiophene, 2-propyl-	64891	001551-27-5	50
4	Cyclohexane, 1-ethyl-2-methyl-, tra	4650	004923-78-8	50
5	1H-Pyrrole-2,5-dione	1156	000541-59-3	47



TD0531.D HANFORD.M Wed Aug 02 14:22:57 1995 HPPC Page

Table 2. Misidentified Analytes with Recommended Name Changes

C-103



. UNKNOWN #.,29,. OF .,100

1. 1,4-Butanediol, dinitrate 180 C4H8N2O6
2. Nitric acid, propyl ester 105 C3H7NO3

Sample file: >TD378 Spectrum #: 996
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	52	3457918	9086	"BIGDB	42	47	1	0	90	16	20	15
2.	52	627134	9219	"BIGDB	36	53	0	0	91	16	20	19

Library Search Compound Report

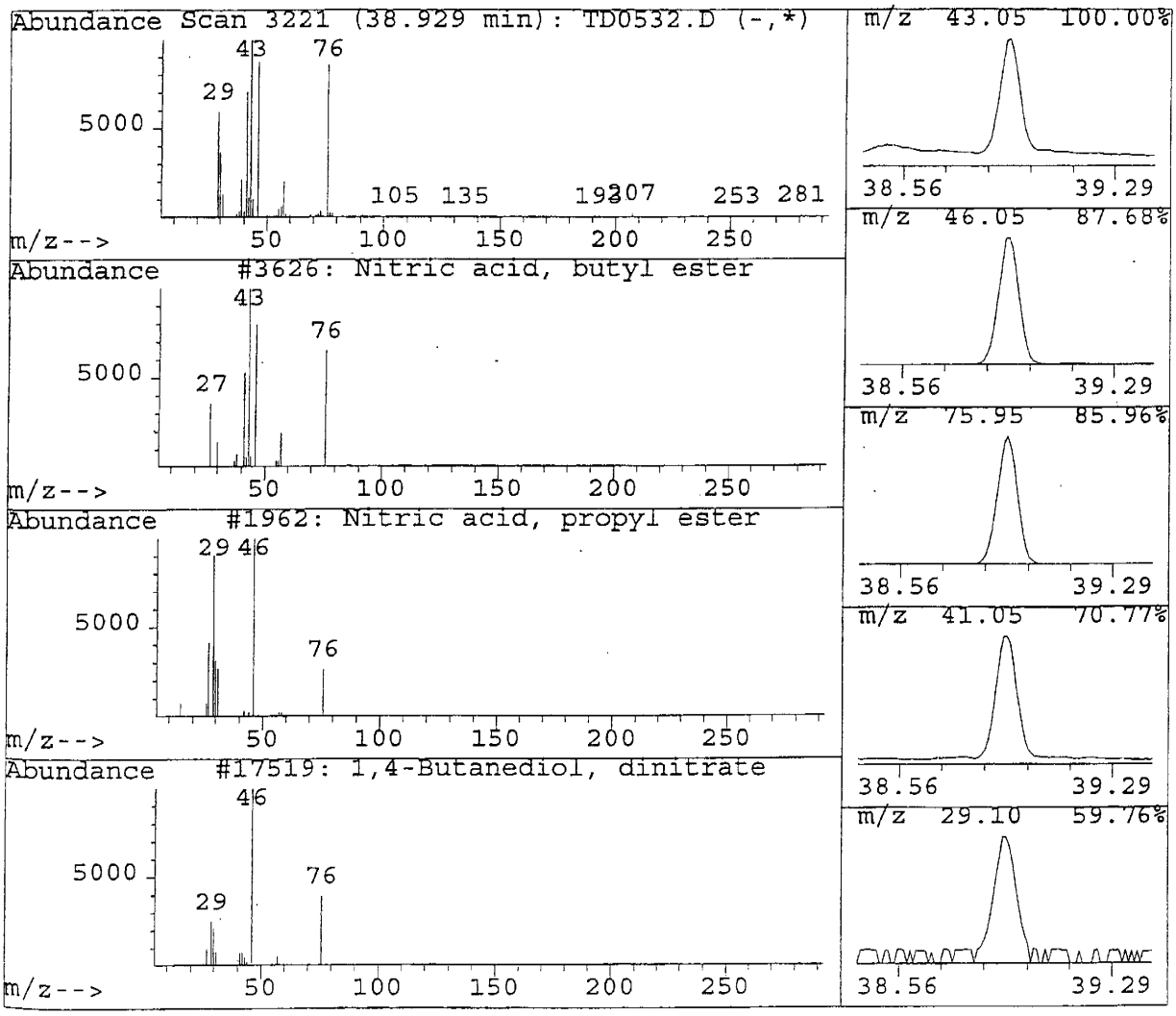
Data File : C:\HPCHEM\1\DATA\TODD\TD0532.D
Acq On : 31 Jul 95 2:28 pm
Sample : TST#1004 AX-102 1.0L
Misc : SAMPLED 6/27/95

Vial: 1
Operator: J.T. SKEEN
Inst : 5972 - In
Multiplr: 1.00

Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

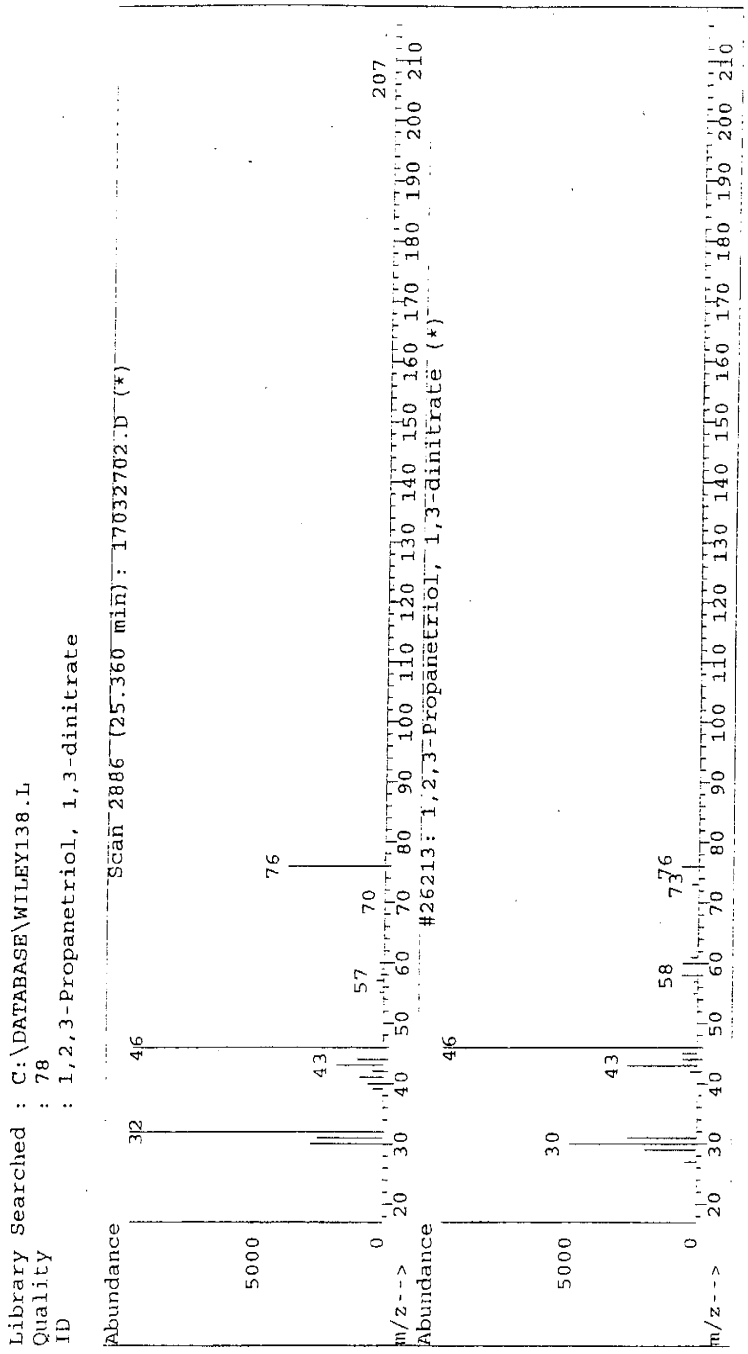
R.T.	Conc	Area	Relative to ISTD	R.T.
38.93	40.20 NG	950524	ETHYLBENZENE-D10	41.47

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	Nitric acid, butyl ester	3626	000928-45-0	78
2	Nitric acid, propyl ester	1962	000627-13-4	72
(3)	1,4-Butanediol, dinitrate	17519	003457-91-8	64
4	Thiourea	62590	000062-56-6	45
5	Carbon disulfide	362	000075-15-0	42

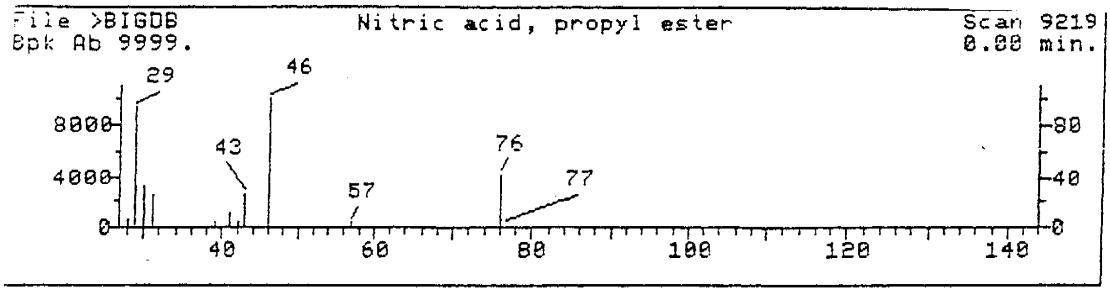


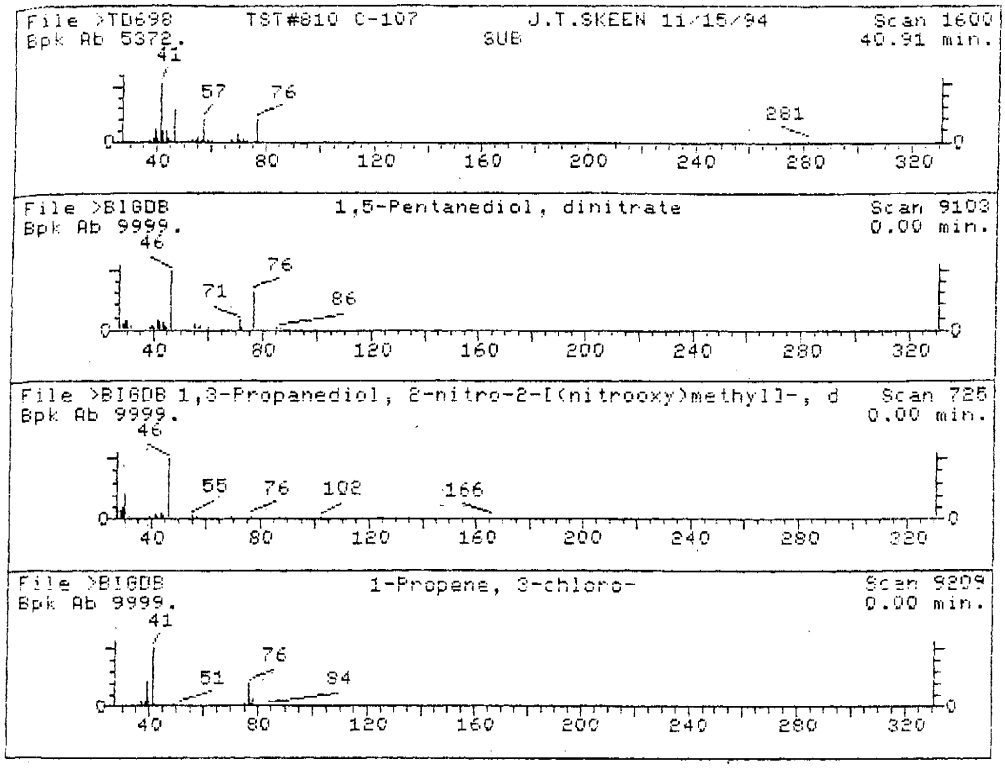
TX-106

V7012-A04-031
3/27/97



2D-40


File >BIGDB
Bpk Ab 9999.
Nitric acid, propyl ester
Scan 9219
0.00 min.
29
46
43
57
76
77
8000
4000
0
80
40
0
40
60
80
100
120
140

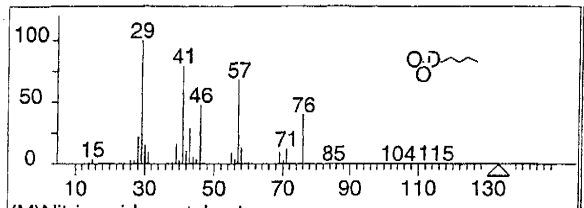


UNKNOWN #.,26,. OF .,89

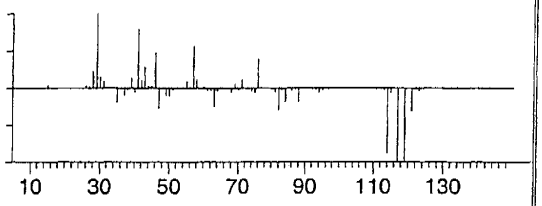
1.	1,5-Pentanediol, dinitrate	194	C5H10N2O6
2.	1,3-Propanediol, 2-nitro-2-[(nitrooxy)methyl]-, dinitrate (ester)	286	C4H6N4O11
3.	1-Propene, 3-chloro-	76	C3H5Cl
4.	1-Propene, 2-chloro-	76	C3H5Cl
5.	Nitric acid, ethyl ester	91	C2H5NO3

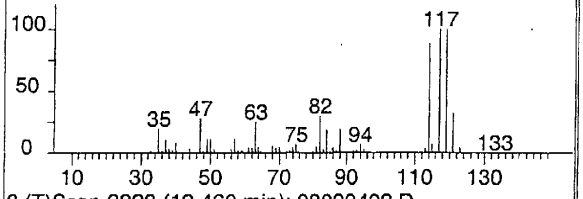
Sample file: >TD698 Spectrum #: 1600
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_I
1.	27	3457929	9103	"BIGDB	29	54	0	0	41	41	6	1
2.	15	20820444	725	"BIGDB	31	59	0	0	38	58	3	1
3.	15*	107051	9209	"BIGDB	25	62	3	0	90	60	3	1
4.	15*	557982	9206	"BIGDB	25	70	3	0	90	58	3	1
5.	15*	625581	9022	"BIGDB	20	66	1	0	156	60	3	1

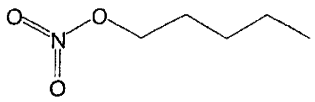


(M)Nitric acid, pentyl ester





? (T)Scan 2223 (12.460 min): 03090402.D

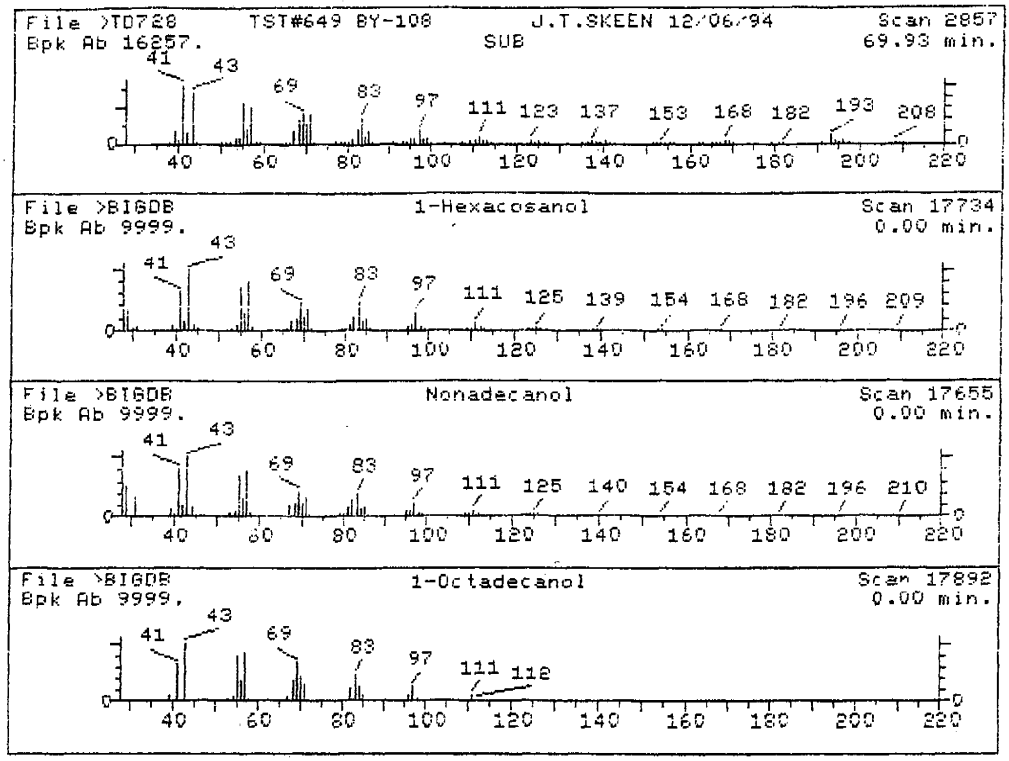


Nitric acid, pentyl ester
Formula: $C_5H_{11}NO_3$
MW: 133 CAS#: 1002-16-0 NIST#: 3127 ID#: 405
DB: mainlib
Other DBs: Fine, RTECS, EINECS
Contributor: MINISTRY OF TECH. E.R.D.E., WALTHAM A
44 Masses and Abundances

12	1	31	95	47	4	60	10
13	1	37	6	50	2	69	95
14	9	38	12	51	3	70	26
15	36	39	157	52	2	71	118
24	2	40	27	53	6	72	7
25	3	41	795	54	6	76	395
26	26	42	102	55	91	77	7
27	29	43	286	56	34	85	4
28	221	44	56	57	680	90	4
29	999	45	32	58	131	104	2
30	150	46	476	59	7	115	3

Synonyms:
1. Amyl nitrate
2. n-Amyl nitrate
3. Amylester kyseliny dusicne
4. Nitrate D'amyle
5. UN 1112

1 (M) Nitric acid, pentyl ester

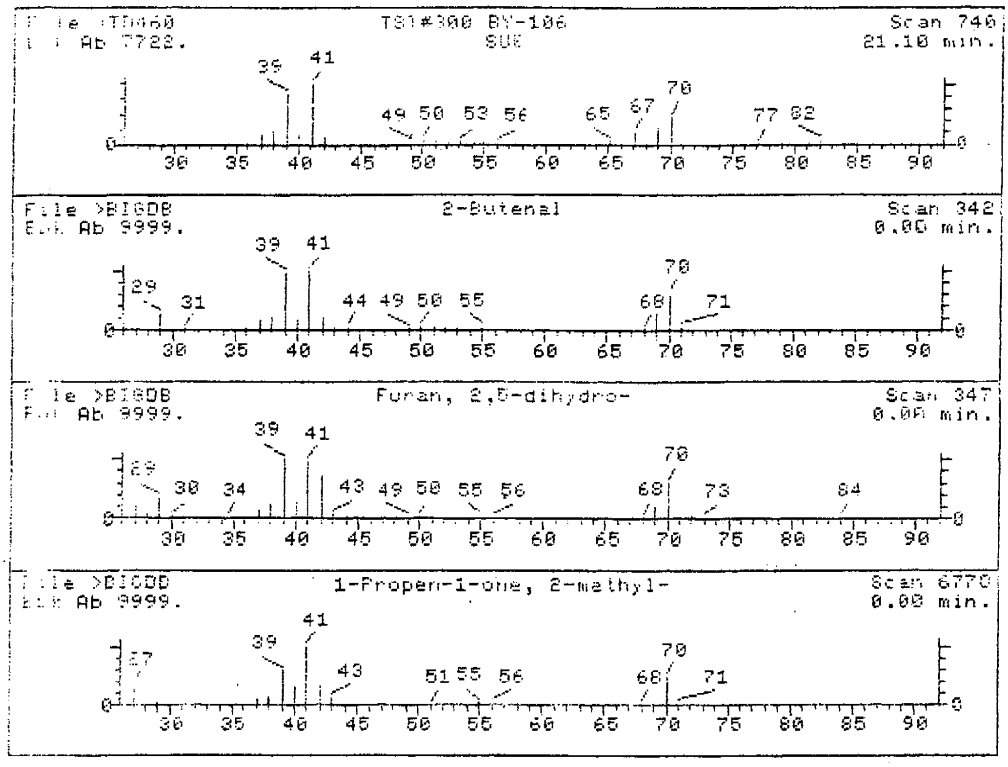


. UNKNOWN #.,164,. OF .,181

1.	1-Hexacosanol	382	C26H54O
2.	Nonadecanol	284	C19H40O
3.	1-Octadecanol	270	C18H38O
4.	1-Eicosanol	298	C20H42O
5.	1-Tetracosanol	354	C24H50O

Sample file: >TD728 Spectrum #: 2857
Search speed: 1 Tilting option: N No. of ion ranges searched: 47

	Prob.	CAS #	CON #	ROOT	K	DR	#FLG	TILT	%	CON	C_i	R_i
1.	67	506525	17734	"BIGDB	115	48	1	0	25	36	28	7
2.	59	52783434	17655	"BIGDB	92	61	1	0	7	4	2	9
3.	54	112925	17892	"BIGDB	84	60	1	0	6	3	2	9
4.	44	6299969	17669	"BIGDB	106	52	2	0	6	3	1	9
5.	44	506514	17720	"BIGDB	100	64	2	0	6	40	1	9



UNKNOWN #.,45,. OF .,2??

1.	2-Butenal	70 C4H6O
(2)	Furan, 2,5-dihydro-	70 C4H6O
3.	1-Propen-1-one, 2-methyl-	70 C4H6O
4.	2,3-DIHYDROFURAN	70 C4H6O
5.	2-Butenal, (E)-	70 C4H6O

Sample file: >TD460 Spectrum #: 740
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	GAS #	COM #	ROOT	K	DH	#F	S	TILT	%	CO	C_	R_
1.	96*	4170303	342	"BIGDB	57	34	2		0	69	16	31	43
2.	60*	12082?8	347	"BIGDB	44	6?	3		0	27	1?	3?	1?
3.	??*	598?65	6??8	"BIGDB	46	47	3		0	100	18	20	17
4.	42*	0	6?62	"BIGDB	28	6?	3		0	79	2?	1?	1?
5.	38*	123??9	?080	"BIGDB	34	65	2		0	40	39	10	14

Library Search Compound Report

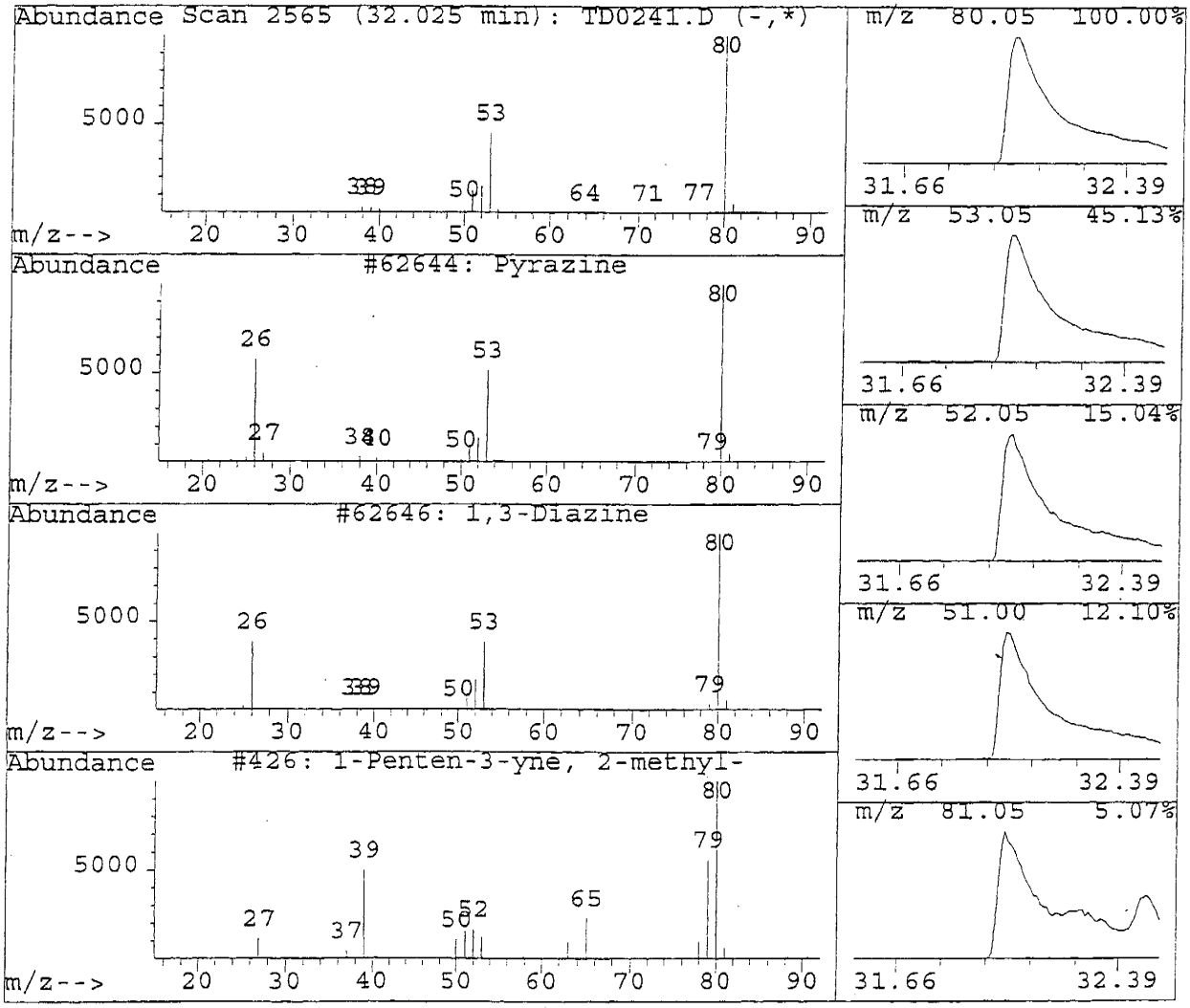
Data File : C:\HPCHEM\1\DATA\TODD\TD0241.D
Acq On : 17 Mar 95 4:10 pm
Sample : TST#526 U-106 2.0L
Misc : SAMPLED 3/07/95

Vial: 1
Operator: J.T. SKEEN
Inst : 5972 - In
Multiplr: 1.00

Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
32.03	347.35 NG	4053962	BENZENE-D6	25.60

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	Pyrazine	62644	000290-37-9	91
2	1,3-Diazine	62646	000289-95-2	90
3	1-Penten-3-yne, 2-methyl-	426	000926-55-6	33
4	s-Triazaborane	62652	006569-51-3	9
5	Pyridazine	415	000289-80-5	7



TD0241.D HANFORD.M Tue Mar 21 17:34:17 1995 HPPC Page 8

Pyrazine good match

Table 3. Misidentified Analytes

Library Search Compound Report

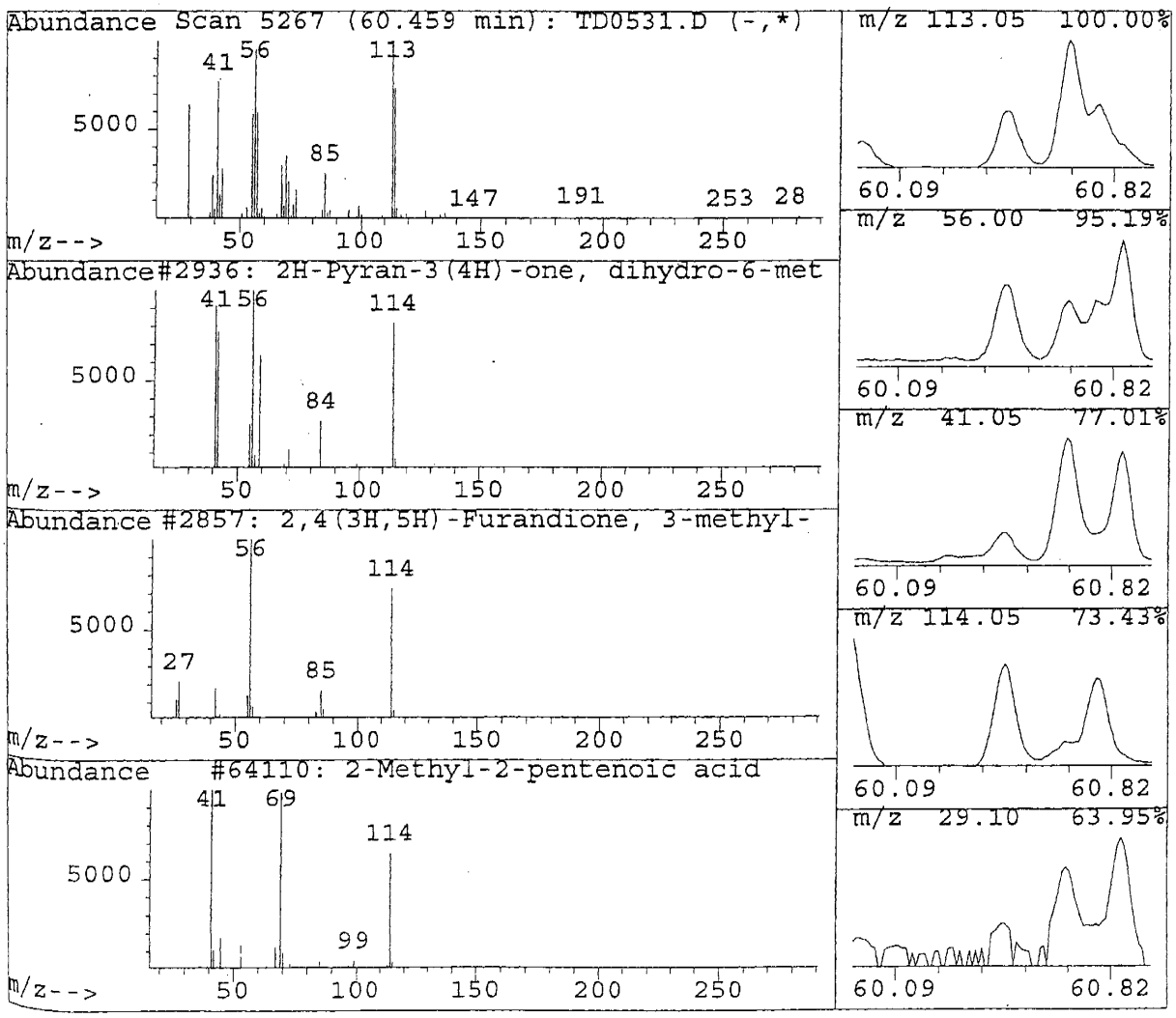
Data File : C:\HPCHEM\1\DATA\TODD\TD0531.D
Acq On : 31 Jul 95 11:56 am
Sample : TST#1003 AX-102 1.0L
Misc : SAMPLED 6/27/95

Vial: 1
Operator: J.T. SKEEN
Inst : 5972 - In
Multiplr: 1.00

Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
60.46	19.54 NG	388469	DODECANE-D26	59.93

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	2H-Pyran-3(4H)-one, dihydro-6-methy	2936	043152-89-2	38
2	2,4(3H,5H)-Furandione, 3-methyl-	2857	001192-51-4	38
3	2-Methyl-2-pentenoic acid	64110	003142-72-1	27
4	Cyclobutanecarboxylic acid, 2,2-dim	4950	042836-66-8	25
5	Piperazine, 1,4-dimethyl-	2952	000106-58-1	22



TD0531.D HANFORD.M Wed Aug 02 14:28:53 1995 HPPC Page 80

Data File: /chem/hpdos1.i/17060802.b/17060809.d

Date : 08-JUN-97 18:58

Client ID: S6118-b30.103

Instrument: hpdos1.i

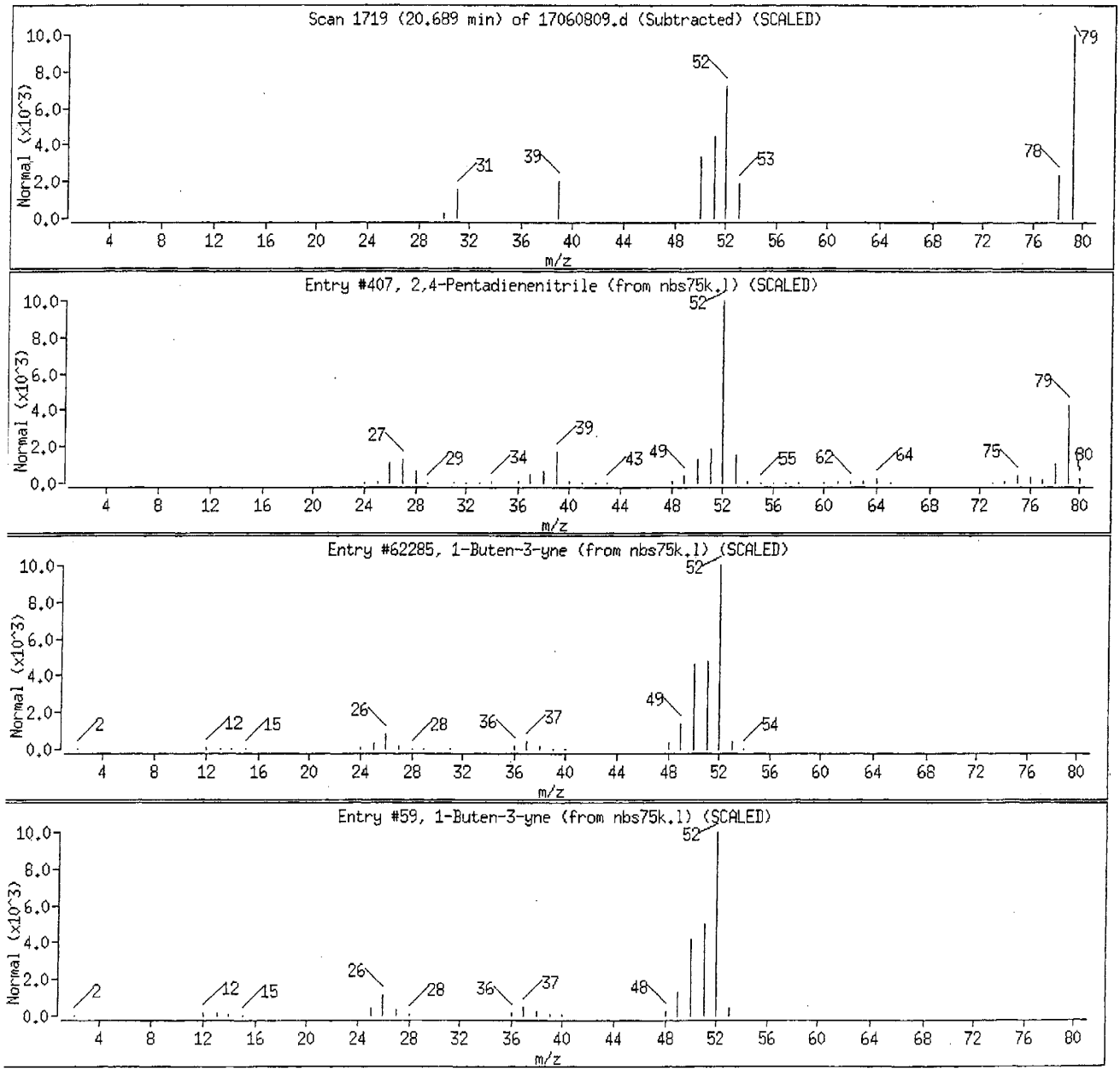
Sample Info: Tank U-112; S6118-b30.103; 100mL;

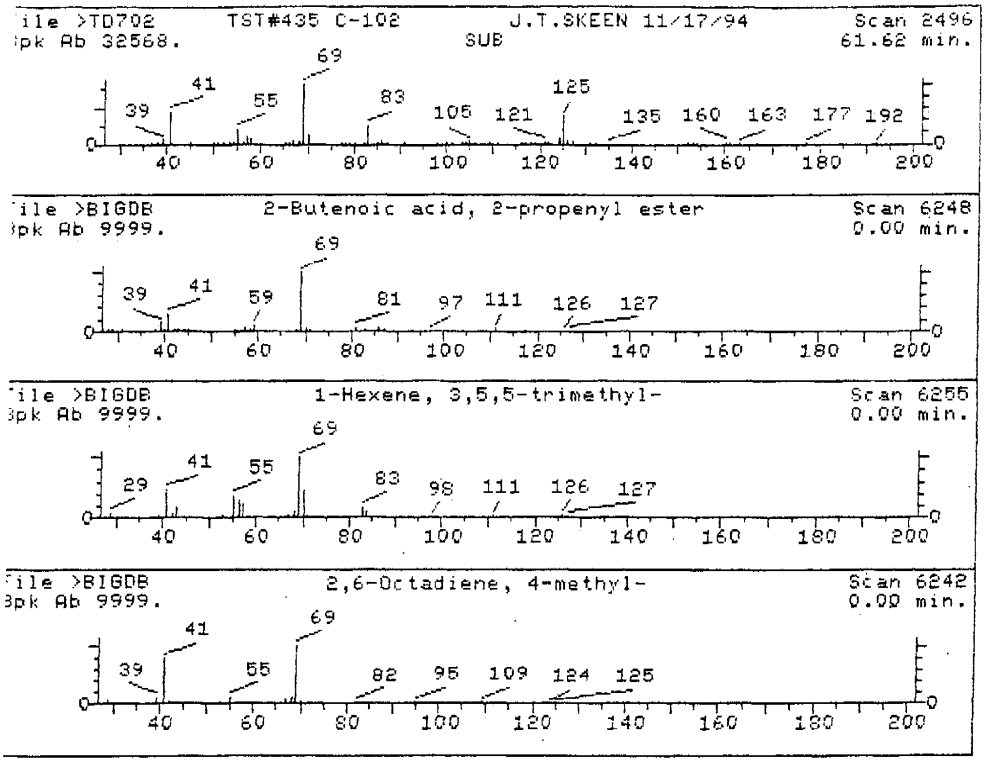
Operator: Alex

Column phase: DB-1

Column diameter: 0.32

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,4-Pentadienenitrile	1615-70-9	nbs75k.l	407	56	C5H5N	79
1-Buten-3-yne	689-97-4	nbs75k.l	62285	5	C4H4	52
1-Buten-3-yne	689-97-4	nbs75k.l	59	5	C4H4	52





UNKNOWN #.,87,. OF .,121

1.	2-Butenoic acid, 2-propenyl ester and others	126 C7H10O2
2.	1-Hexene, 3,5,5-trimethyl-	126 C9H18
3.	2,6-Octadiene, 4-methyl-	124 C9H16
4.	1,5-HEPTADIENE, 3,4-DIMETHYL-, CIS=TRANS	124 C9H16
5.	2,6-HEPTADIENE, 2,5-DIMETHYL-	124 C9H16

Sample file: >TD702 Spectrum #: 2496
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	25*	20474935	6248	"BIGDB	22	53	3	0	100	46	7	12
2.	24*	4316658	6255	"BIGDB	24	69	3	0	100	42	8	12
3.	20*	74498945	6242	"BIGDB	35	43	2	0	69	52	5	17
4.	20*	0	6245	"BIGDB	31	42	2	0	76	52	5	15
5.	20*	0	6246	"BIGDB	32	50	3	0	70	52	5	14

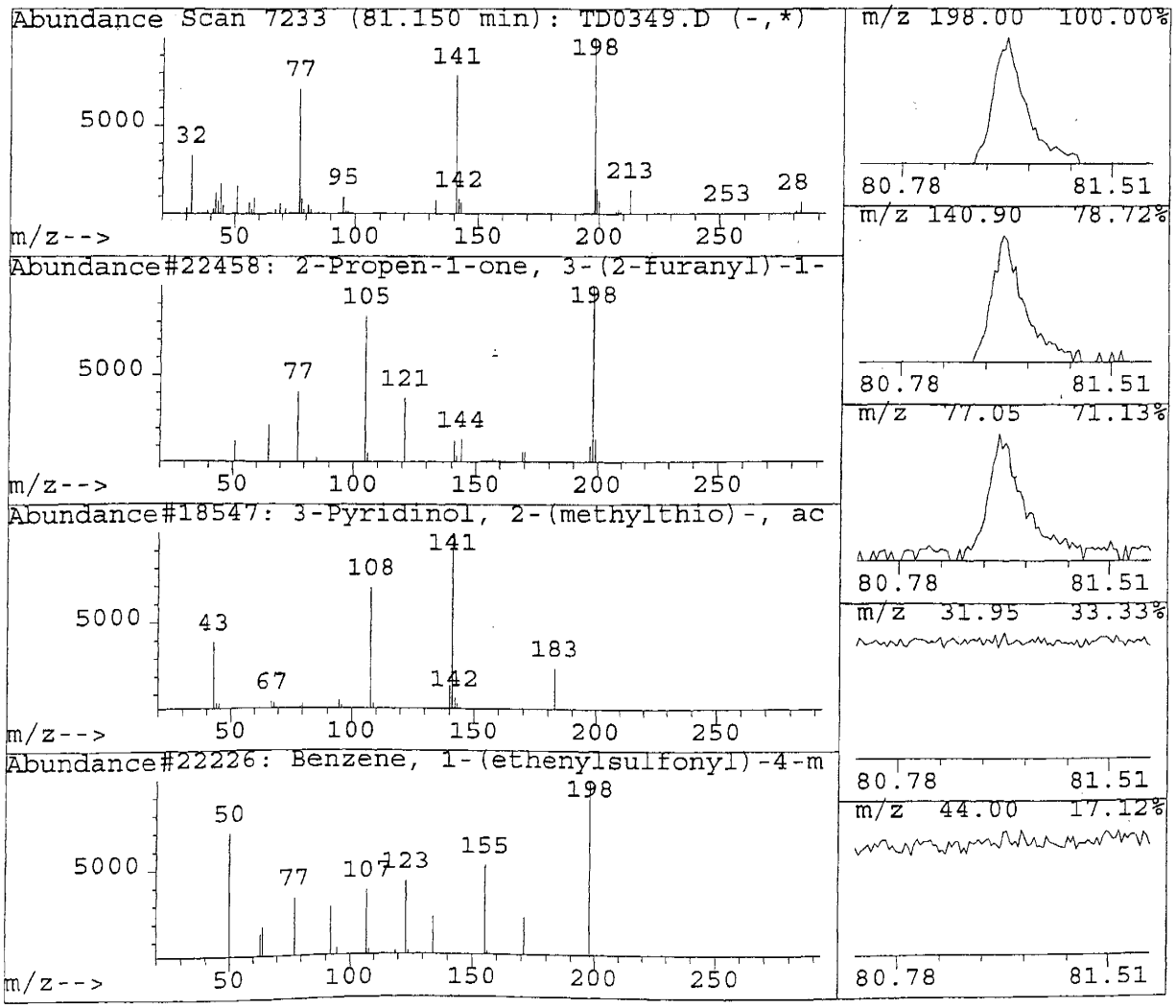
Data File : C:\HPCHEM\1\DATA\TODD\TD0349.D
Acq On : 25 Apr 95 10:16 am
Sample : TST#496 SX-106 1.0L
Misc : SAMPLED 3/24/95

Vial: 1
Operator: J.T. SKEEN
Inst : 5972 - In
Multiplr: 1.00

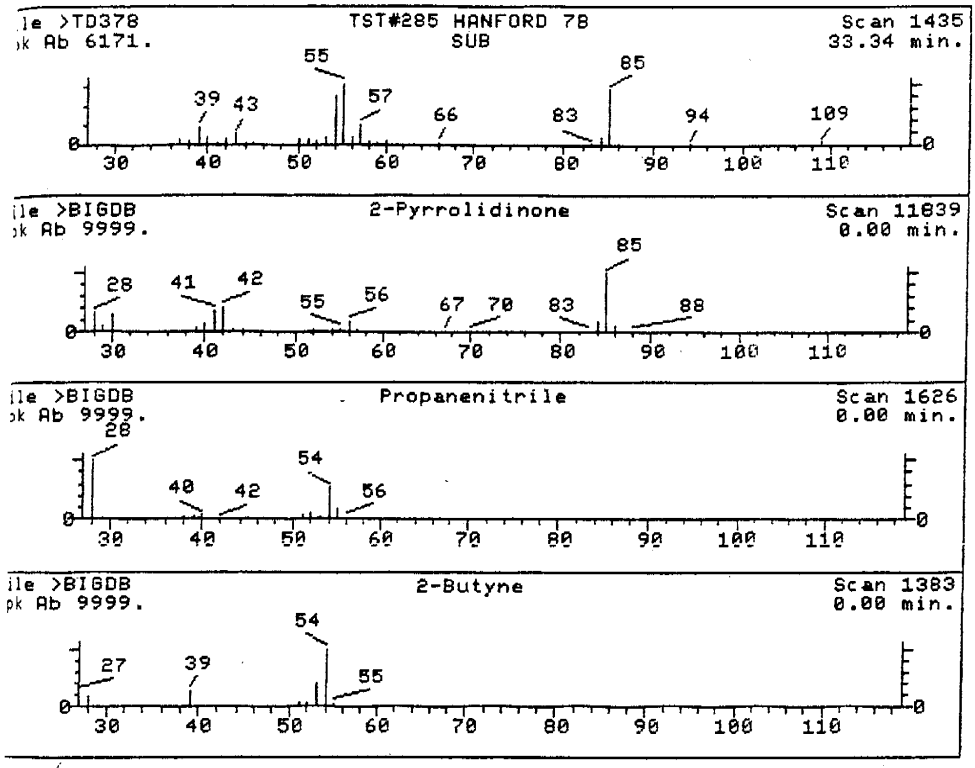
Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
81.15	5.13 NG	105737	DODECANE-D26	59.00

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	2-Propen-1-one, 3-(2-furanyl)-1-phenyl	22458	000717-21-5	25
2	3-Pyridinol, 2-(methylthio)-, aceta	18547	042715-30-0	10
3	Benzene, 1-(ethenylsulfonyl)-4-meth	22226	016191-87-0	9
4	Dibenzothiophene, 3-methyl-	22461	016587-52-3	9
5	1,2,3,4-Tetramethoxybenzene	22278	000000-00-0	9



C-103

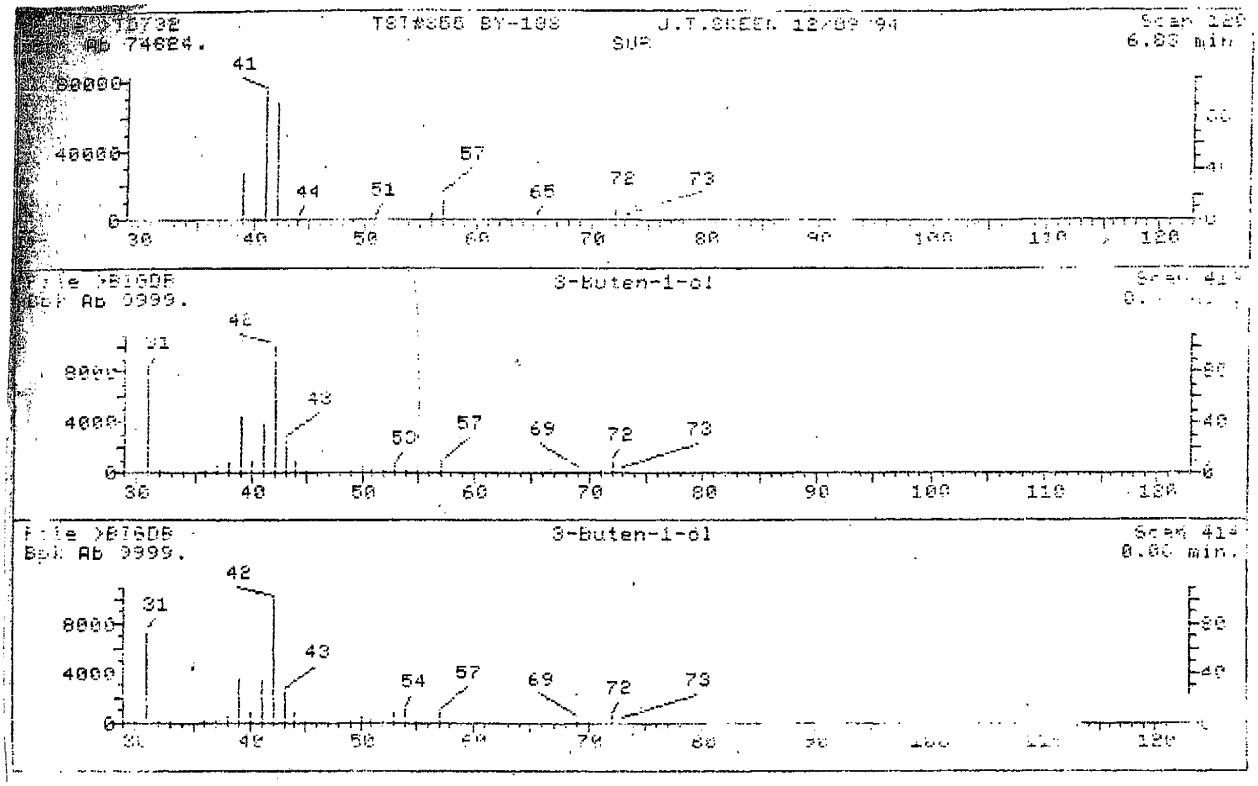


UNKNOWN #.,52,. OF .,100

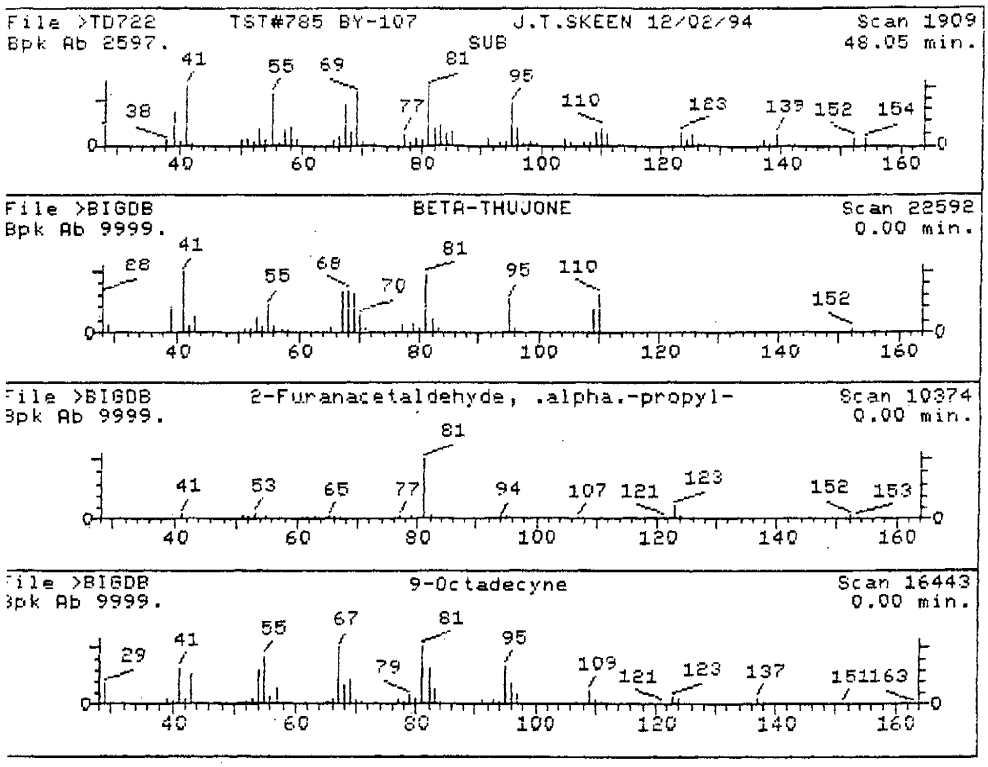
1.	2-Pyrrolidinone	85 C4H7NO
2.	Propanenitrile	55 C3H5N
3.	2-Butyne	54 C4H6
4.	1-AZA-1,3-BUTADIEN	55 C3H5N
5.	Ethenamine, N-methylene-	55 C3H5N

Sample file: >TD378 Spectrum #: 1435
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	26*	616455	11839	"BIGDB	27	63	2	0	69	45	8	14
2.	20*	107120	1626	"BIGDB	28	58	1	0	81	55	5	15
3.	15*	503173	1383	"BIGDB	24	42	1	0	75	60	3	14
4.	15*	0	1389	"BIGDB	30	56	2	0	100	57	3	15
5.	15*	38239279	1388	"BIGDB	30	56	2	0	100	57	3	15


TST#388 BY-108
J.T.GREEN 12/09/94
SUR
6.83 min
Ab 74624.
41
44
51
57
65
72
73
3-Buten-1-ol
Bpk Ab 9999.
31
42
43
50
57
69
72
73
3-Buten-1-ol
Bpk Ab 9999.
0.00 min.
31
42
43
54
57
69
72
73

Q. 3-Buten-1-ol



. UNKNOWN #.,88,. OF .,183

1.	BETA-THUJONE	152	C10H16O
2.	2-Furanacetaldehyde, .alpha.-propyl-	152	C9H12O2
3.	9-Octadecyne	250	C18H34
4.	2,4-Decadienal, (E,E)-	152	C10H16O
5.	2,4-Decadienal, (E,Z)-	152	C10H16O

Sample file: >TD722 Spectrum #: 1909
Search speed: 1 Tilting option: N No. of ion ranges searched: 55

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	51*	0	22592	"BIGDB	69	52	3	0	100	34	20	35
2.	40*	31681262	10374	"BIGDB	37	46	0	0	98	50	12	42
3.	35	353655944	16443	"BIGDB	70	86	3	0	69	28	14	12
4.	32*	251528454	10376	"BIGDB	42	62	0	0	94	54	9	44
5.	32*	251528344	10375	"BIGDB	41	63	0	0	98	52	9	43

Library Search Compound Report

Data File : C:\HPCHEM\1\DATA\TODD\TD0306.D
Acq On : 11 Apr 95 10:11 am
Sample : TST#846 U-105 1.0L
Misc : SAMPLED 2/24/95

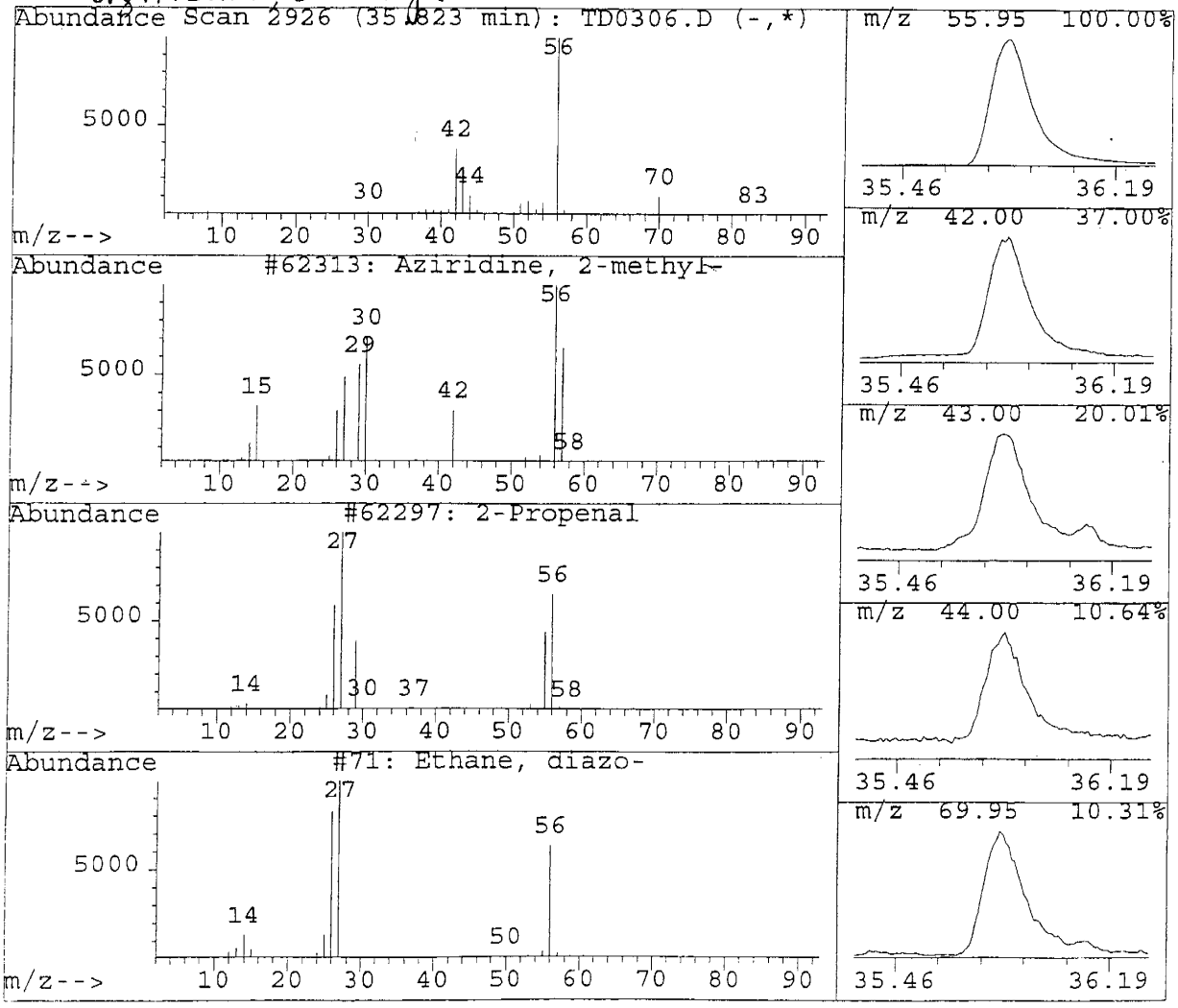
Vial: 1
Operator: J.T. SKEEN
Inst : 5972 - In
Multiplr: 1.00

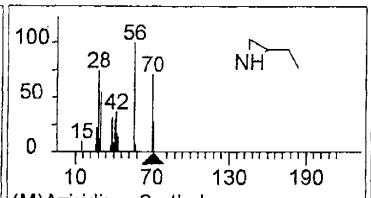
Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
35.82	89.75 NG	1655443	ETHYLBENZENE-D10	40.45

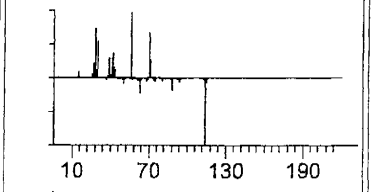
Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	Aziridine, 2-methyl-	62313	000075-55-8	4
2	2-Propenal	62297	000107-02-8	3
3	Ethane, diazo-	71	001117-96-0	3
4	Oxirane, (1-methylethyl)-	721	001438-14-8	2
5	Cyclobutanecarbonitrile, 3,3-dimeth	2221	053783-86-1	2

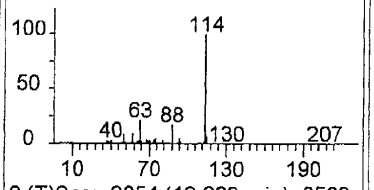
aziridine, 2-ethyl -



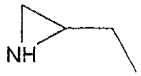


(M)Aziridine, 2-ethyl-





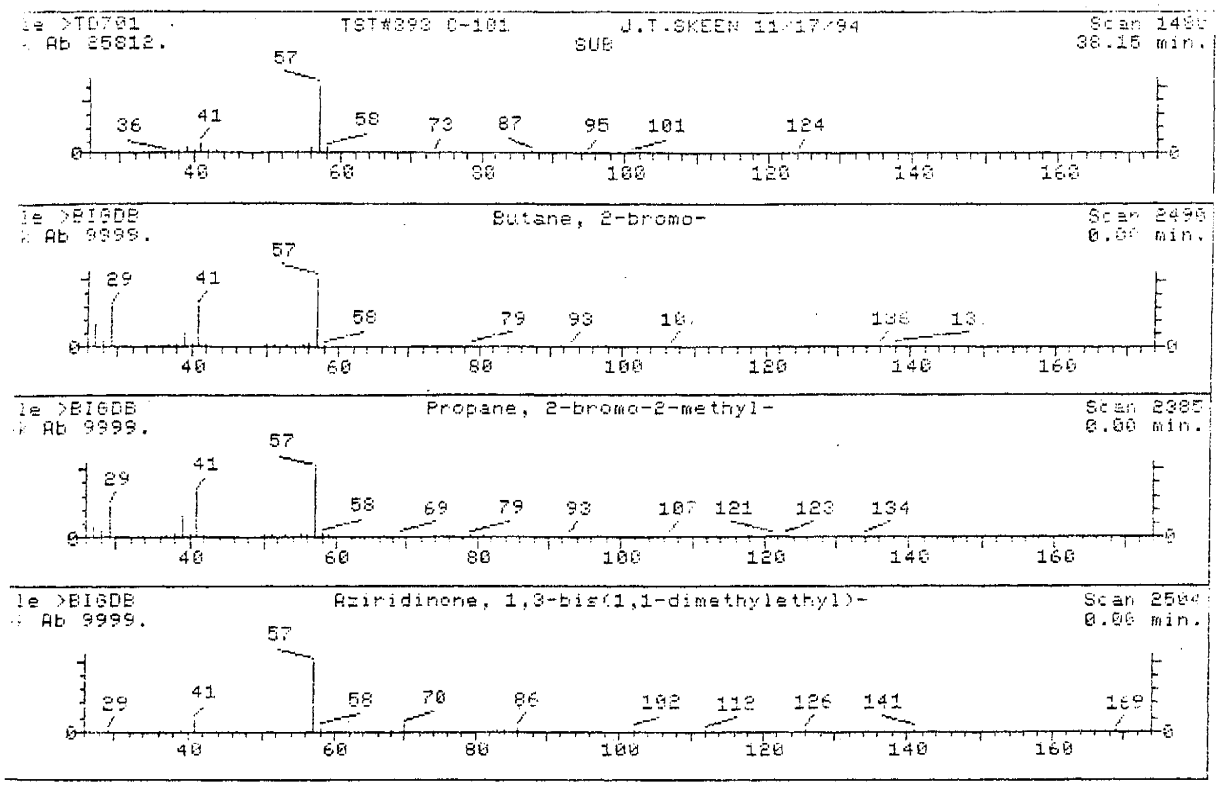
? (T)Scan 2054 (12.663 min): 0509



Formula:
MW: CAS#:
NIST#: ID#:
DB:
Other DBs:

Masses			
15		41	
26		42	
27		43	
28		44	
29		56	
30		57	
38		70	
39		71	
40		72	

Synonyms:
1.
2.
3.
4.
5.
6.



Butane - 2- bromo

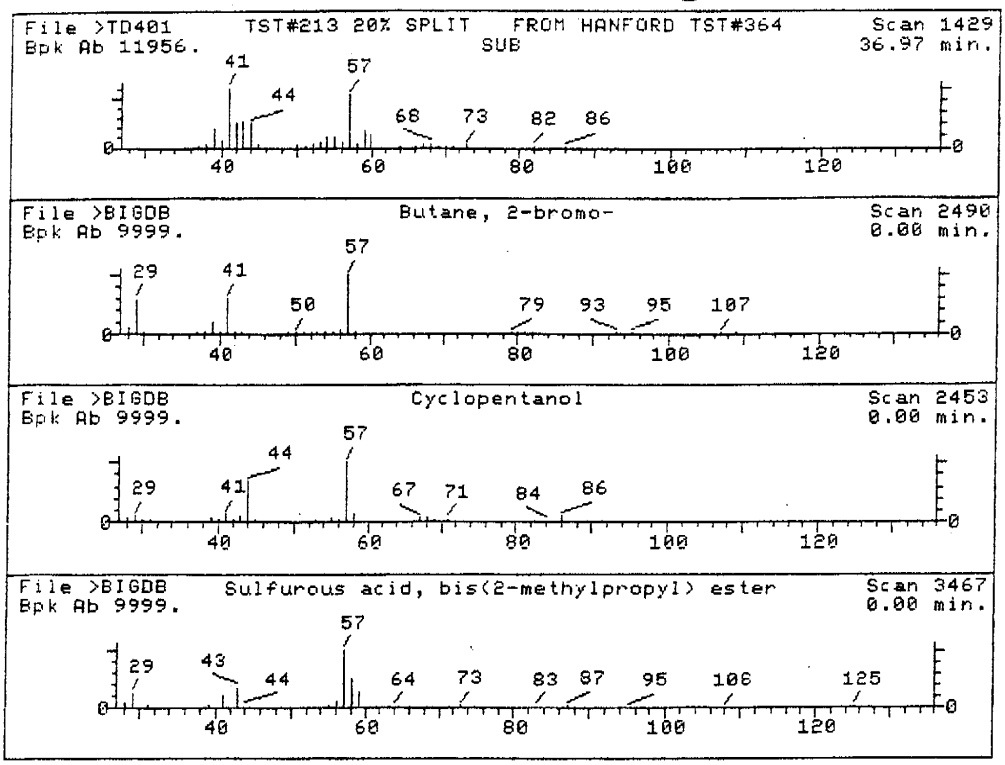
UNKNOWN #.,38,. OF .,11

1.	Butane, 2-bromo-	136	C4H9Br
2.	Propane, 2-bromo-2-methyl-	136	C4H9Br
3.	Aziridinone, 1,3-bis(1,1-dimethylethyl)-	169	C10H19NO
4.	Butane, 1,1'-oxybis-	130	C8H18O
5.	Butane, 1,1'-oxybis-	130	C8H18O

Sample file: >TD701 Spectrum #: 1480
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROUT	K	DK	#F	S	TILT	%	COR	C_I	R_IV
1.	62*	78762	2490	"BIGDB	51	29	1		0	71	26	25	43
2.	45	507197	2389	"BIGDB	45	34	1		0	68	23	12	16
3.	43*	14387894	2504	"BIGDB	25	44	2		0	100	21	17	14
4.	35	142961	13812	"BIGDB	35	40	2		0	86	26	14	12
5.	35	142961	13810	"BIGDB	36	42	2		0	70	28	14	12

C-103

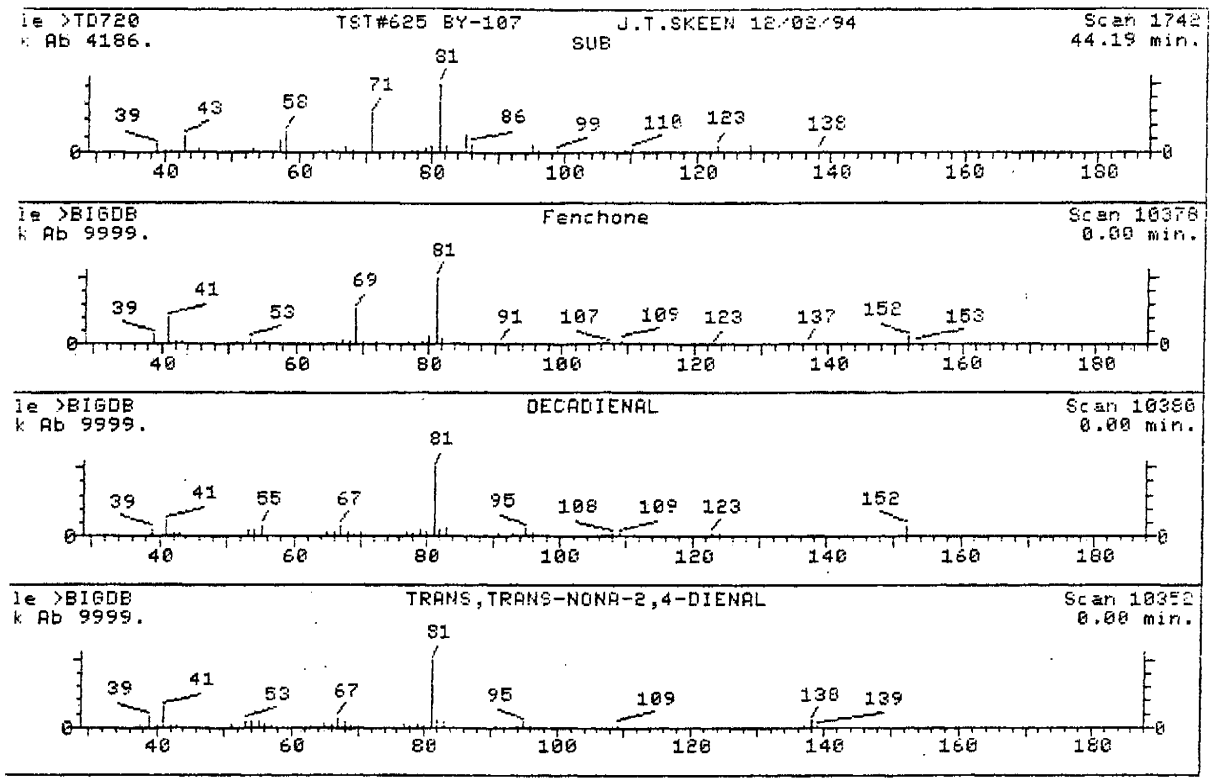


. UNKNOWN #.,30,. OF .,141

√1.	Butane, 2-bromo-	136 C4H9Br
√2.	Cyclopentanol	86 C5H10O
3.	Sulfurous acid, bis(2-methylpropyl) ester	194 C8H18O3S
4.	Butane, 1-(2-methoxyethoxy)-	132 C7H16O2
5.	Propane, 1-bromo-2-methyl-	136 C4H9Br

Sample file: >TD401 Spectrum #: 1429
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	26*	78762	2490	"BIGDB	41	39	0	0	89	60	7	53
2.	25	96413	2453	"BIGDB	39	42	2	0	61	46	7	13
3.	20	18748271	3467	"BIGDB	35	56	1	0	89	54	5	12
4.	20*	13343981	3273	"BIGDB	30	69	2	0	89	52	5	14
5.	15	78773	2387	"BIGDB	38	42	1	0	89	57	3	14



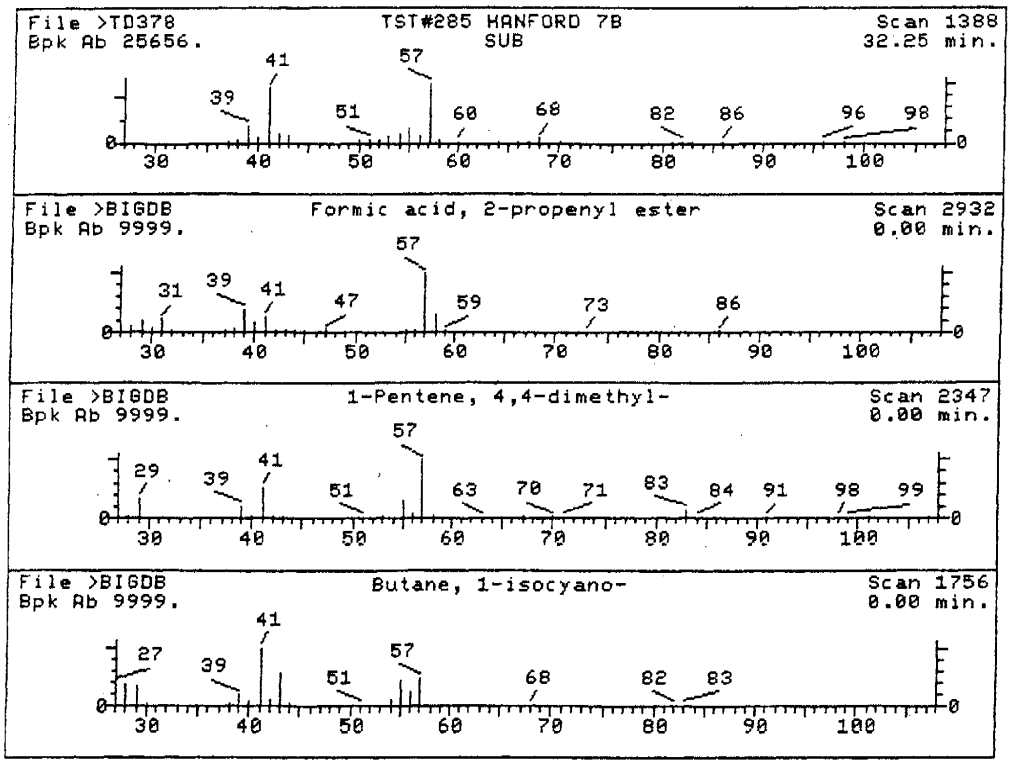
UNKNOWN #.,62,. OF .,175

1.	Fenchone	152	C10H16O
2.	DECADIENAL	152	C10H16O
3.	TRANS,TRANS-NONA-2,4-DIENAL	138	C9H14O

Sample file: >TD720 Spectrum #: 1742
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#F	S	TILT	%	CO	C_	R_I
1.	20	1195795	10378	"BIGDB	41	46	2		0	78	53		13
2.	20	0	10380	"BIGDB	42	49	2		0	76	55		
3.	15	0	10352	"BIGDB	40	48	2		0	81	56		

C-103

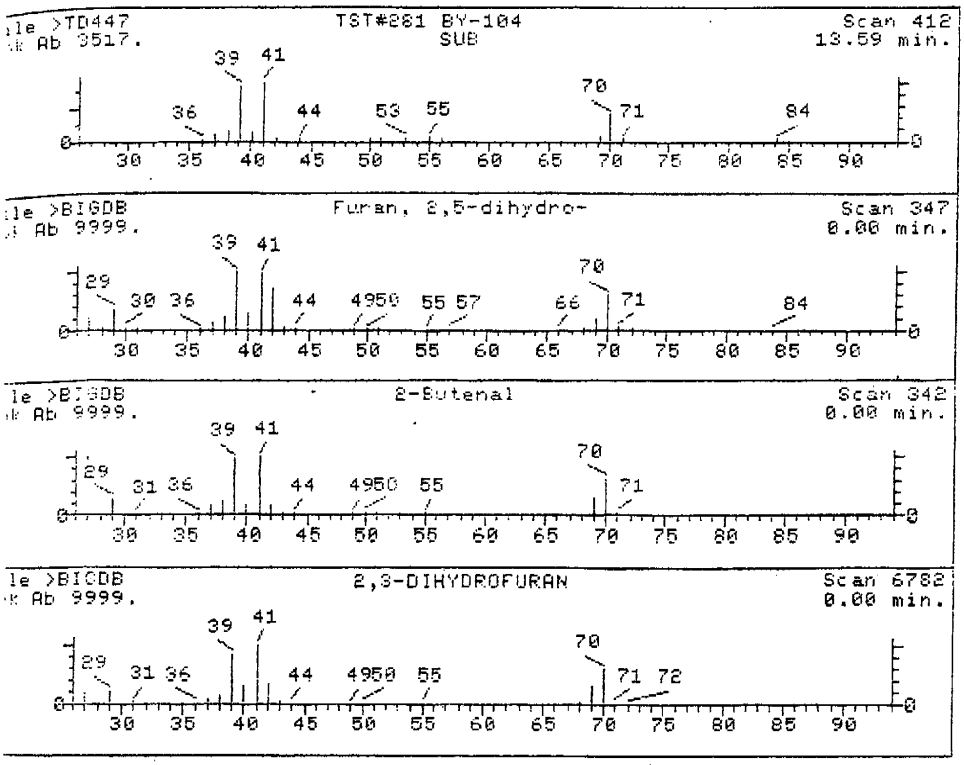


UNKNOWN #.,49,. OF .,100

1.	Formic acid, 2-propenyl ester	86 C4H6O2
2.	1-Pentene, 4,4-dimethyl-	98 C7H14
3.	Butane, 1-isocyano-	83 C5H9N

Sample file: >TD378 Spectrum #: 1388
Search speed: 1 Tilting option: N No. of ion ranges searched: 51

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	43*	1838591	2932	"BIGDB	28	58	2	0	72	23	17	14
2.	37*	762629	2347	"BIGDB	25	51	1	0	76	27	14	14
3.	20*	2769644	1756	"BIGDB	24	60	3	0	92	51	5	12

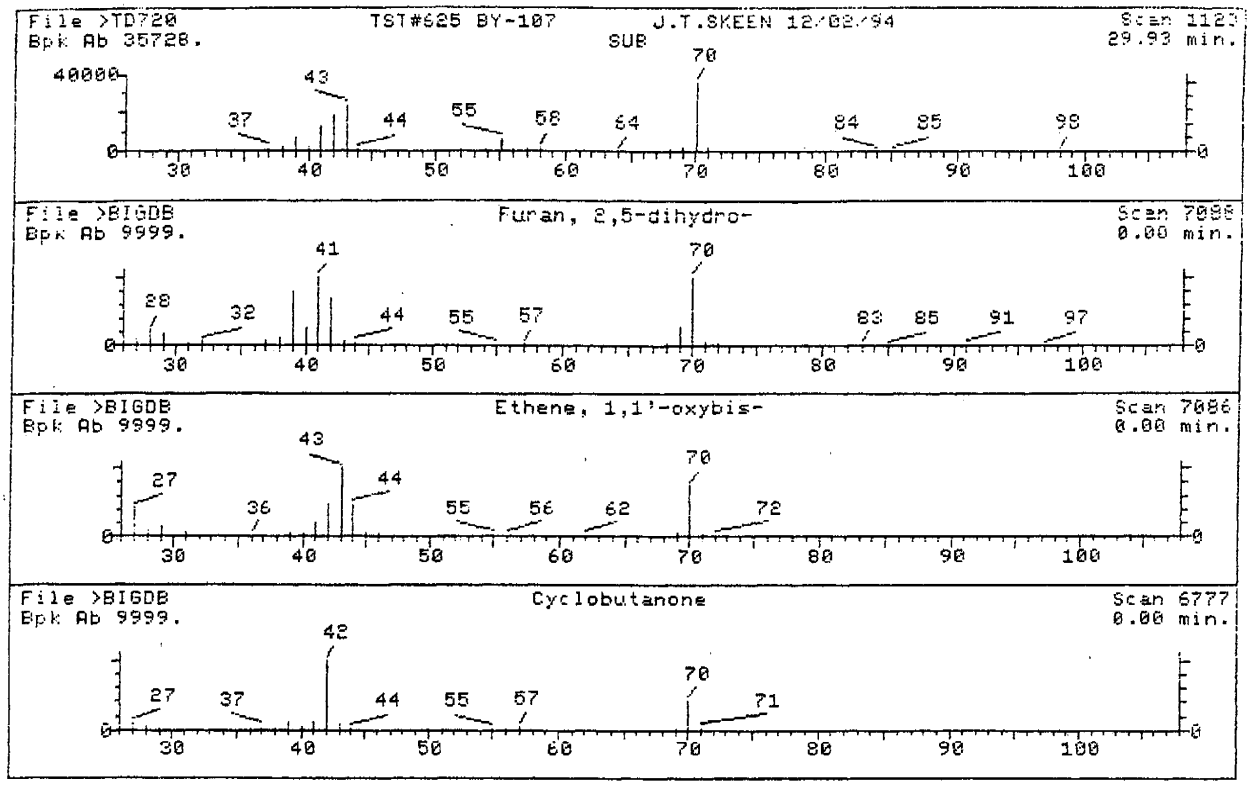


UNKNOWN #.,22,. OF .,237

1.	Furan, 2,5-dihydro-	70 C4H6O
2.	2-Butenal	70 C4H6O
3.	2,3-DIHYDROFURAN	70 C4H6O
4.	CYCLOPROPANE CARBOXALDEHYDE	70 C4H6O
5.	2-Butenal, (E)-	70 C4H6O

Sample file: >TD447 Spectrum #: 412
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	COR	C_	R_IN
1.	70*	1708298	347	"BIGDB	49	62	3	0	75	10	42	13
2.	67*	4170303	342	"BIGDB	48	43	2	0	70	13	34	2E
3.	60*	0	6782	"BIGDB	34	60	3	0	77	15	30	13
4.	37*	0	316	"BIGDB	32	65	2	0	100	27	14	14
5.	31*	123739	7080	"BIGDB	35	79	2	0	51	33	12	14



UNKNOWN #.,29,. OF .,175

1.	Furan, 2,5-dihydro-	70	C4H6O
2.	Ethene, 1,1'-oxybis-	70	C4H6O
3.	Cyclobutanone	70	C4H6O
4.	1-Pentene	70	C5H10
5.	Azetidine, 2-methyl-	71	C4H9N

Sample file: >TD720 Spectrum #: 1123
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROUT	K	DK	#FwG	TILT	%	CON	C_I	R_IU
1.	70*	1708298	7088	"BIGDB	30	69	3	0	77	9	42	13
2.	52*	109933	7086	"BIGDB	25	63	3	0	111	20	20	13
3.	27*	1191953	6777	"BIGDB	22	48	2	0	238	36	10	13
4.	26*	109671	7104	"BIGDB	24	57	3	0	210	36	10	12
5.	20*	19812498	7112	"BIGDB	34	64	3	0	52	55	5	13

Data File: /chem/hpdos1.i/17061202.b/17061204.d

Date : 12-JUN-97 17:41

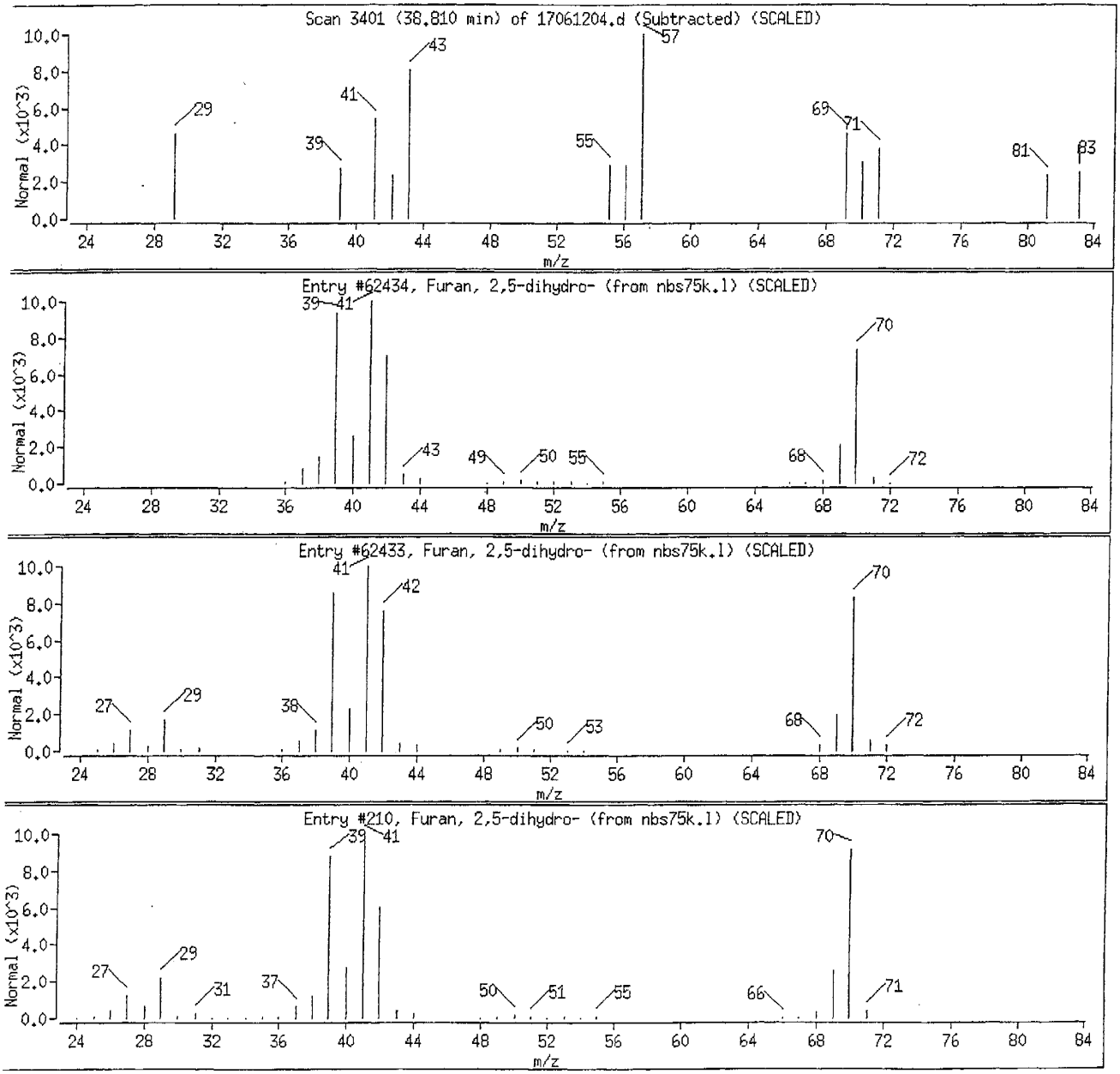
Client ID: S6119-t39.309 Instrument: hpdos1.i

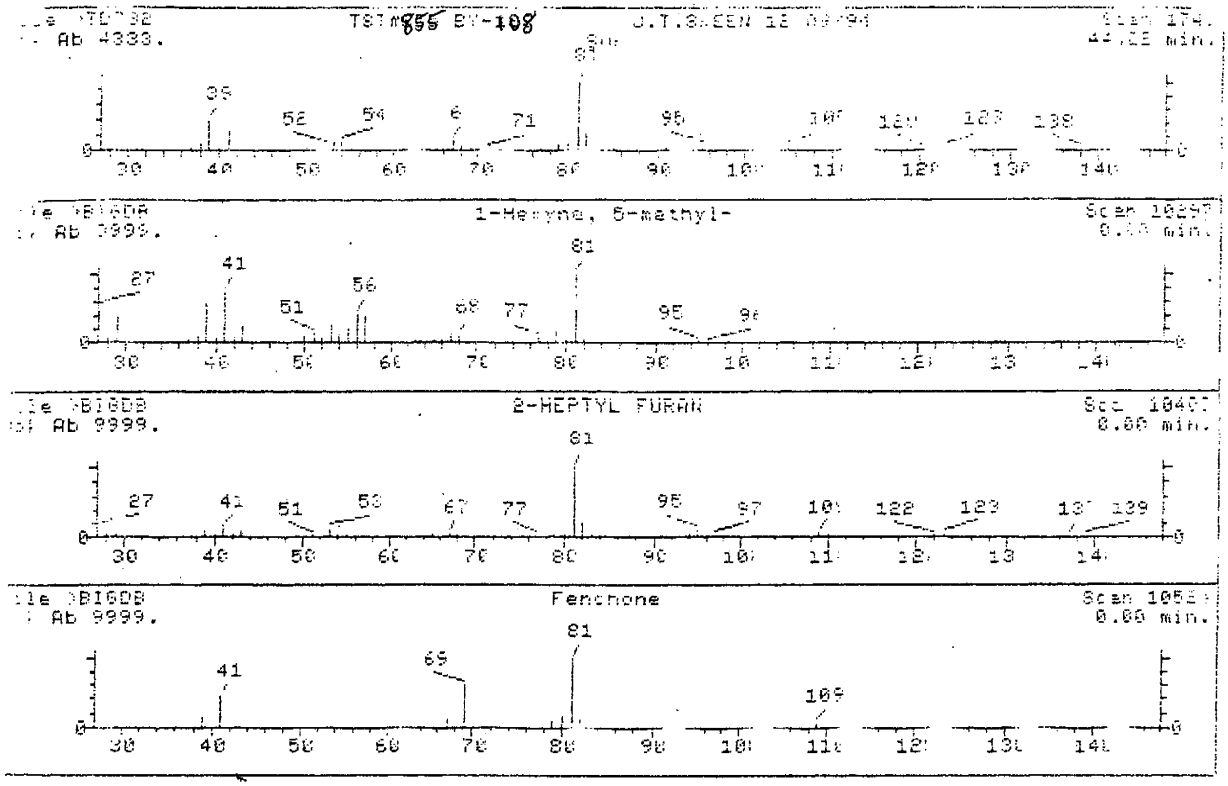
Sample Info: Tank U-112; S6119-t39.309; 100mL

Operator: Alex

Column phase: DB-1 Column diameter: 0.32

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Furan, 2,5-dihydro-	1708-29-8	nbs75k.l	62434	9	C4H6O	70
Furan, 2,5-dihydro-	1708-29-8	nbs75k.l	62433	9	C4H6O	70
Furan, 2,5-dihydro-	1708-29-8	nbs75k.l	210	9	C4H6O	70





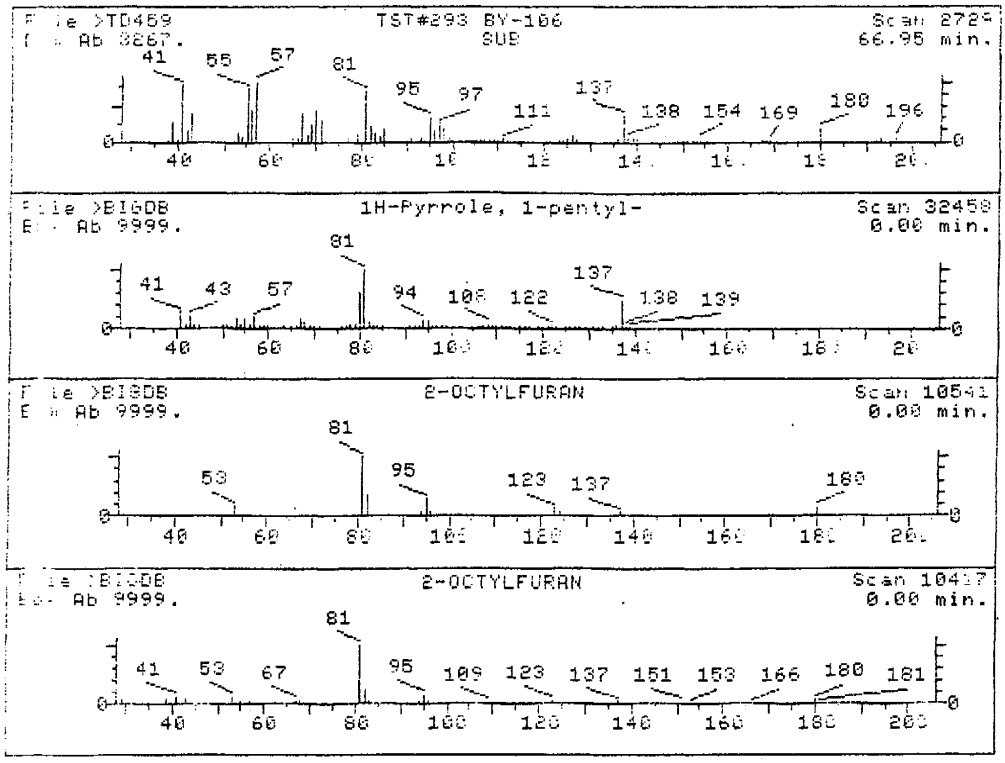
UNKNOWN #.,72,. OF .,1

1. 1-Hexyne, 5-methyl-
2. 2-HEPTYL FURAN
3. Fenchone
4. 1H-Pyrrole, 1-methyl-
5. CYCLOPENTENE, 3-ACETYL-3-METHYL-

96 C
166 C11H18O
152 C10H16O
81 C5H7N
124 C8H12O

Sample file: >TD732 Spectrum #: 1743
Search speed: 1 Tilting option: N No. of mass ranges searched: 1

	Prob.	CAS #	COMPOUND #	RCD	K	DF	#F	TIC	%	CO	C_	M_
1.	72*	2200[illegible]07	10297	[illegible]DB	94	72	3	0	75	25	17	[illegible]
2.	27	0	10018	[illegible]DB	47	47	[illegible]	0	100	34	16	[illegible]
3.	27	1195[illegible]95	10924	[illegible]DB	80	57	[illegible]	0	69	40	10	[illegible]
4.	26*	96948	10[illegible]46	[illegible]DB	34	57	[illegible]	0	100	47	[illegible]	[illegible]
5.	26*	0	10337	[illegible]DB	23	46	2	0	74	47	[illegible]	[illegible]

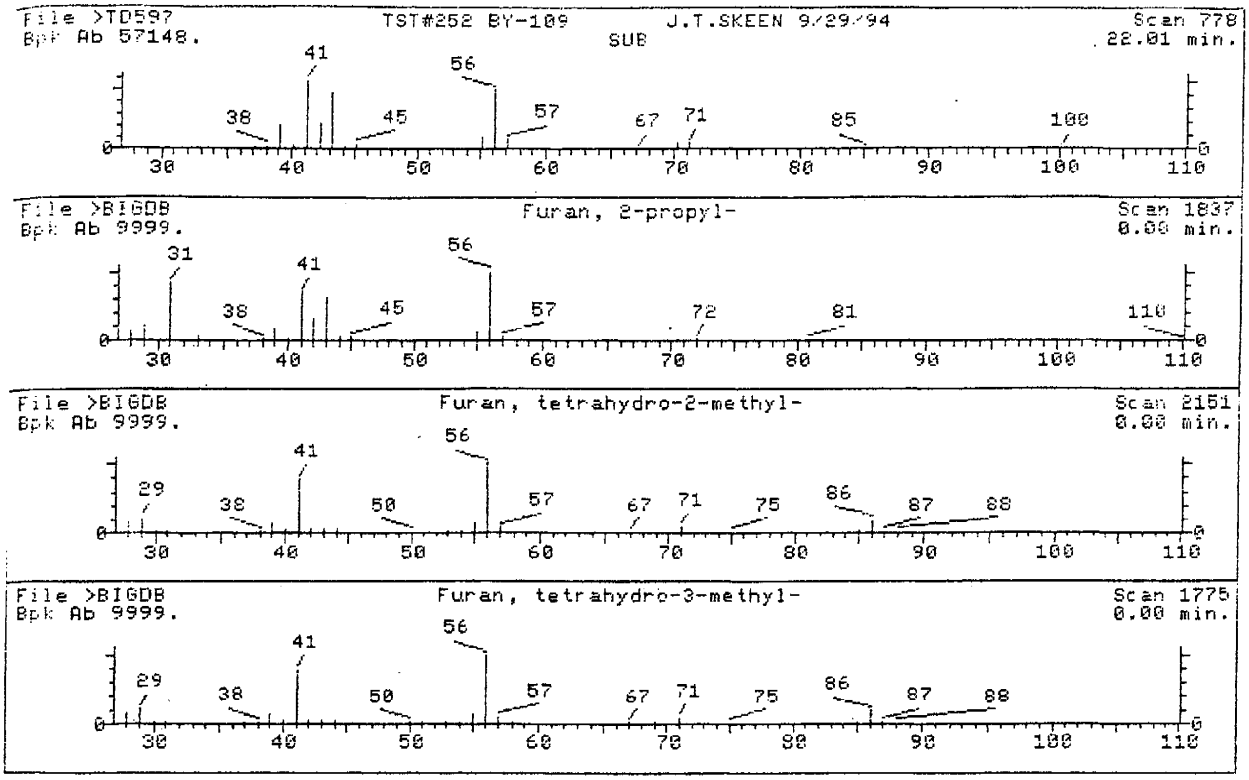


UNKNOWN #.,191,. OF .,2??

1.	1H-Pyrrole, 1-pentyl-	137 C9H15N
(2)	2-OCTYLFURAN	180 C12H20O
3.	2-OCTYLFURAN	180 C12H20O
4.	1,3-Benzodioxole, 2-ethenylhexahydro-	154 C9H14O2

Sample file: >TD459 Spectrum #: 2729
Search speed: 1 Tilting option: N No. of ion ranges searched: 4?

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	F_IV
1.	20*	699229	32458	"BIGDB	36	70	3	0	83	53	5	13
2.	16*	0	10541	"BIGDB	22	49	2	0	74	58	3	13
3.	11*	0	10417	"BIGDB	37	58	2	0	83	65	2	16
4.	11*	55702631	10391	"BIGDB	41	75	2	0	58	65	2	14

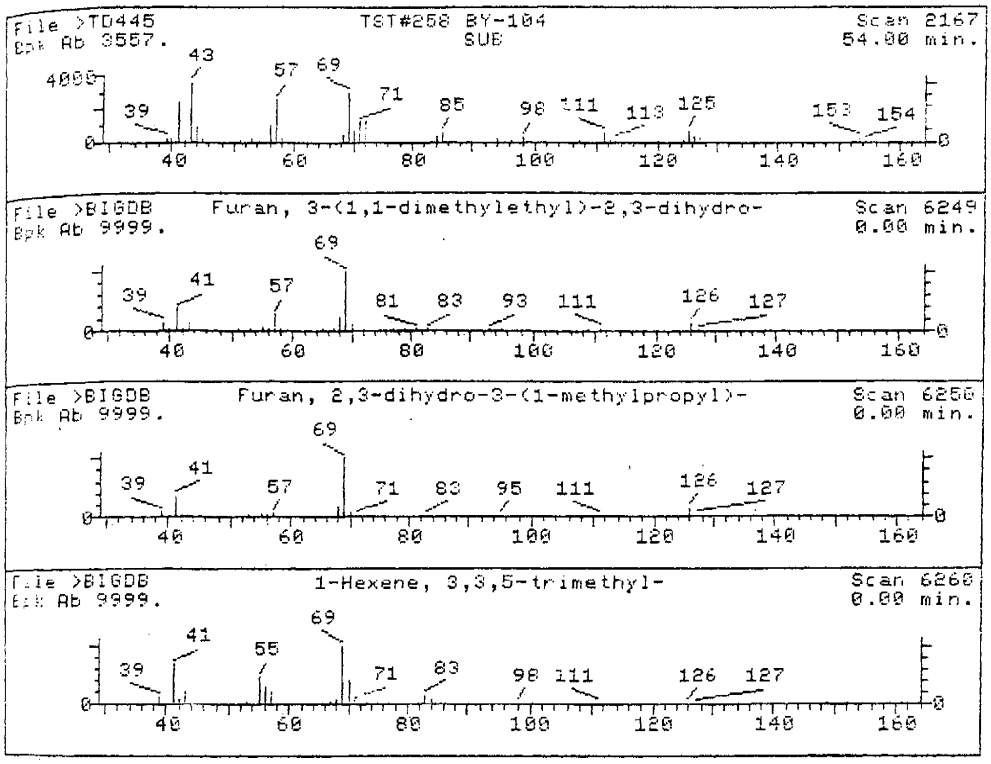


. UNKNOWN #.,12,. OF .,8

1.	Furan, 2-propyl-	110	C7H10O
2.	Furan, tetrahydro-2-methyl-	86	C5H10O
3.	Furan, tetrahydro-3-methyl-	86	C5H10O
4.	Oxetane, 2,3,4-trimethyl-, (2.alpha.,3.alpha.,4.beta.)-	100	C6H12O
5.	Cyclobutane	56	C4H8

Sample file: >TD597 Spectrum #: 778
Search speed: 1 Tilting option: N No. of ion ranges searched: 4

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	36	4229918	1837	"BIGDB	36	54	1	0	83	29	14	13
2.	20	96479	2151	"BIGDB	37	43	2	0	87	53	5	12
3.	20	13423159	1775	"BIGDB	37	43	2	0	87	53	5	12
4.	20*	32347129	1823	"BIGDB	26	51	1	0	87	52	5	14
5.	11*	287230	1743	"BIGDB	29	56	2	0	86	63	2	14

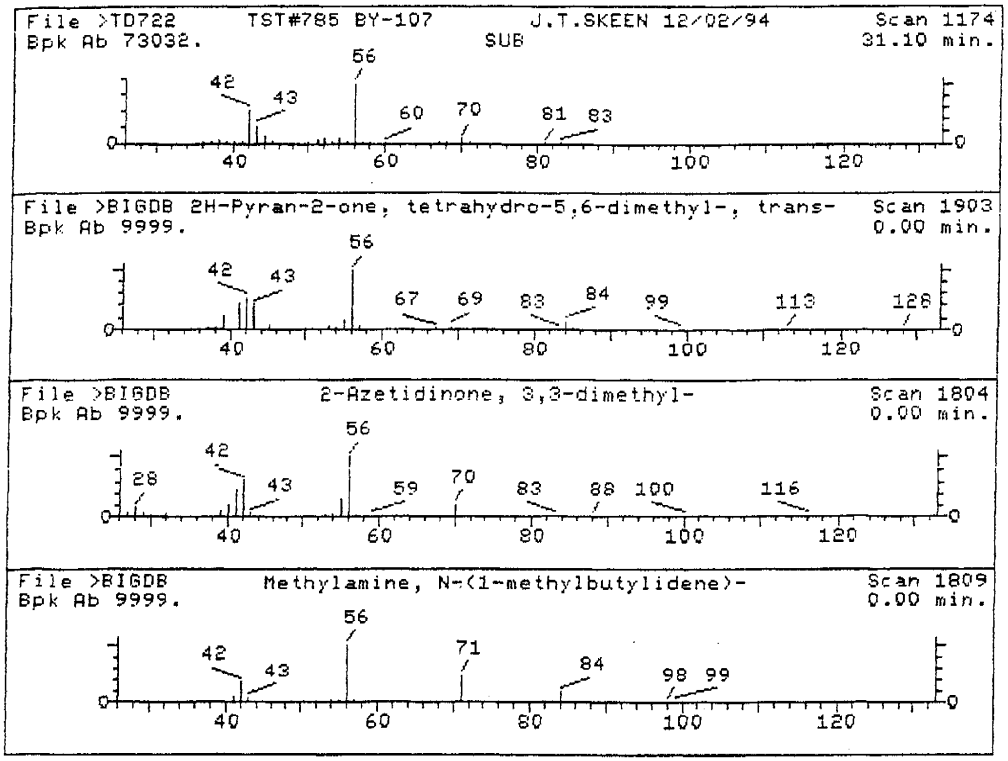


UNKNOWN #.,163,. OF .,265

1.	Furan, 3-(1,1-dimethylethyl)-2,3-dihydro-	126	C8H140
2.	Furan, 2,3-dihydro-3-(1-methylpropyl)-	126	C8H140
3.	1-Hexene, 3,3,5-trimethyl-	126	C9H18
4.	1,6-OCTADIENE, 3,5-DIMETHYL-, CIS	138	C10H18
5.	1-Pentene, 3,3-dimethyl-	98	C7H14

Sample file: >TD445 Spectrum #: 2167
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#F.G	TILT	%	CON	C_	R_IU
1.	25*	34314824	6249	"BIGDB	27	57	2	0	60	47	7	14
2.	25*	56805324	6250	"BIGDB	22	55	2	0	70	48	7	13
3.	25*	13427435	6260	"BIGDB	26	66	3	0	84	50	7	13
4.	20	0	6281	"BIGDB	35	45	2	0	84	52	5	12
5.	20*	3404737	6184	"BIGDB	26	57	3	0	84	51	5	13



UNKNOWN #.,43,. OF .,183

1.	2H-Pyran-2-one, tetrahydro-5,6-dimethyl-, trans-	128	C7H12O2
2.	2-Azetidinone, 3,3-dimethyl-	99	C5H9NO
3.	Methylamine, N-(1-methylbutylidene)-	99	C6H13N
4.	Butane, 1-chloro-	92	C4H9Cl

Sample file: >TD722 Spectrum #: 1174
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_I
1.	67*	24405161	1903	"BIGDB	41	42	2	0	72	14	34	2
2.	60*	7486911	1804	"BIGDB	24	61	2	0	89	12	30	1
3.	36*	22431090	1809	"BIGDB	23	56	2	0	100	28	14	1
4.	31*	109693	2177	"BIGDB	28	58	2	0	100	33	12	1

Library Search Compound Report

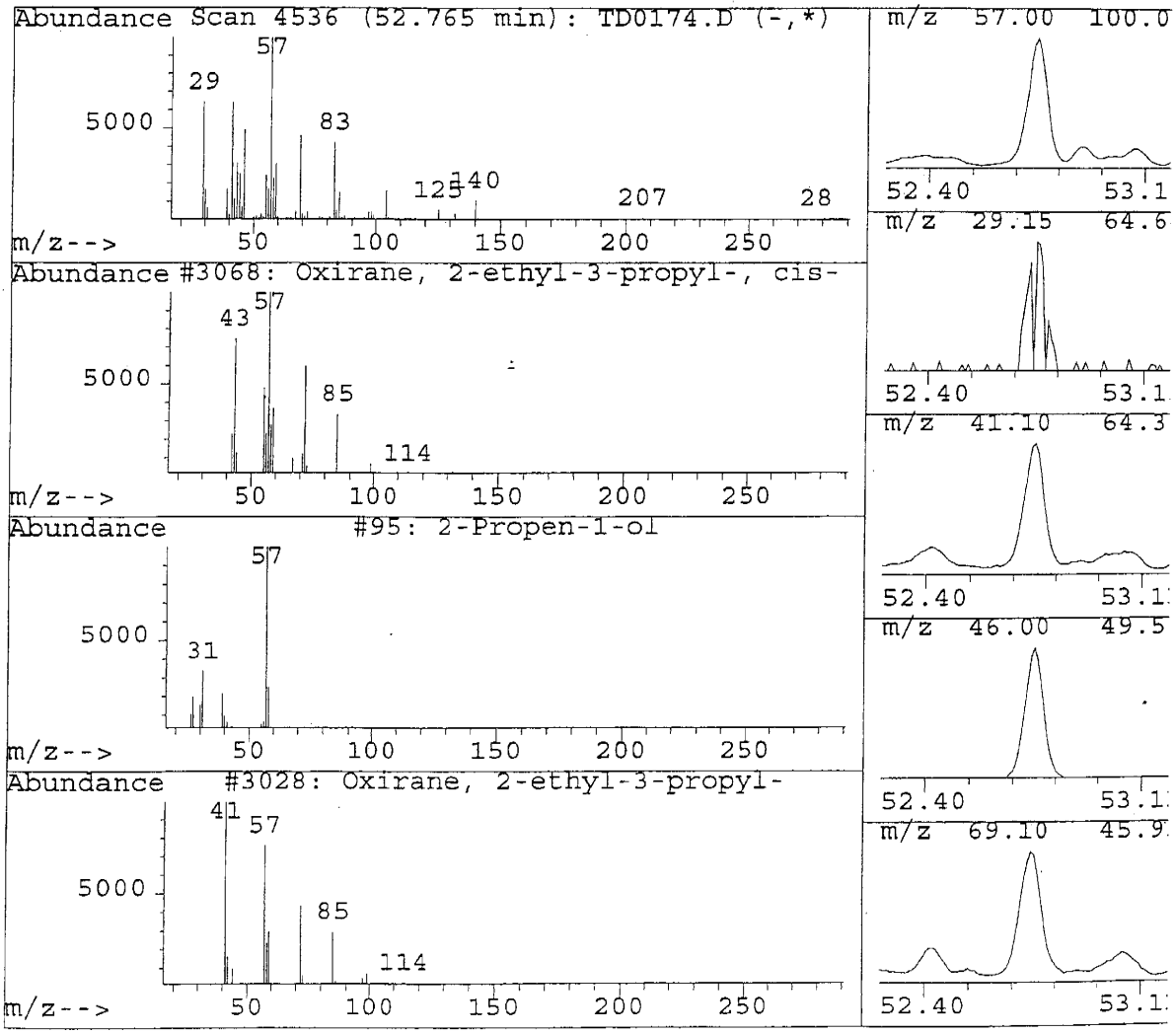
Data File : C:\HPCHEM\1\DATA\TODD\TD0174.D
Acq On : 16 Feb 95 5:32 pm
Sample : TST#565 BX-104 200 ML
Misc : SAMPLED 12/30/94

Vial: 1
Operator: J.T
Inst : 597
Multiplr: 1.0

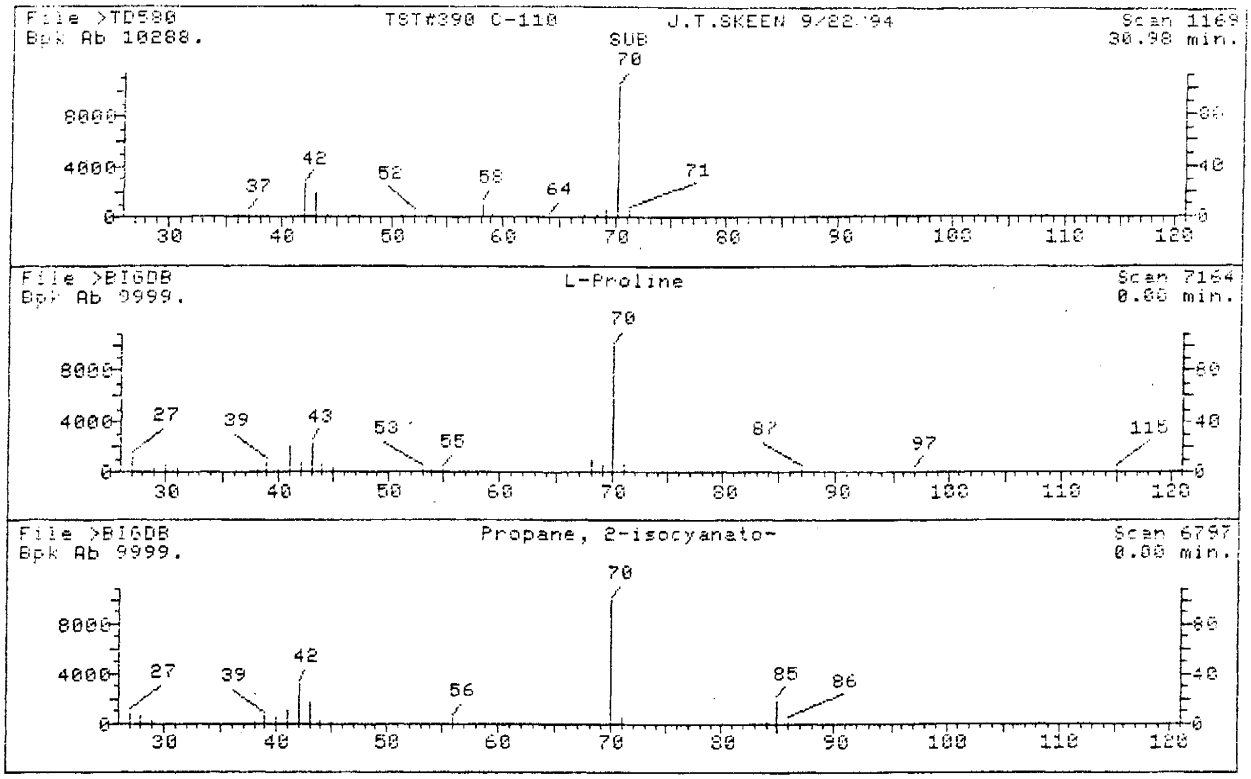
Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
52.77	32.14 NG	826385	DODECANE-D26	59.58

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	Oxirane, 2-ethyl-3-propyl-, cis-	3068	056052-94-9	10
2	2-Propen-1-ol	95	000107-18-6	9
3	Oxirane, 2-ethyl-3-propyl-	3028	053897-32-8	9
4	L-Cysteine, N-(trifluoroacetyl)-, b	51199	005282-99-5	9
5	2H-Pyran, 2-(1,1-dimethylethoxy)tet	11931	001927-69-1	9



TD0174.D HANFORD.M Fri Feb 17 07:43:00 1995 HPPC Pa



. UNKNOWN #.,21,. OF .,156

1. L-Proline — 115 C5H9NO2
2. Propane, 2-isocyanato- — 85 C4H7NO

Sample file: >TD580 Spectrum #: 1169
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	38*	147853	7164	"BIGDB	30	47	2	0	84	28	14	15
2.	35	1795488	6797	"BIGDB	36	40	2	0	81	28	14	12

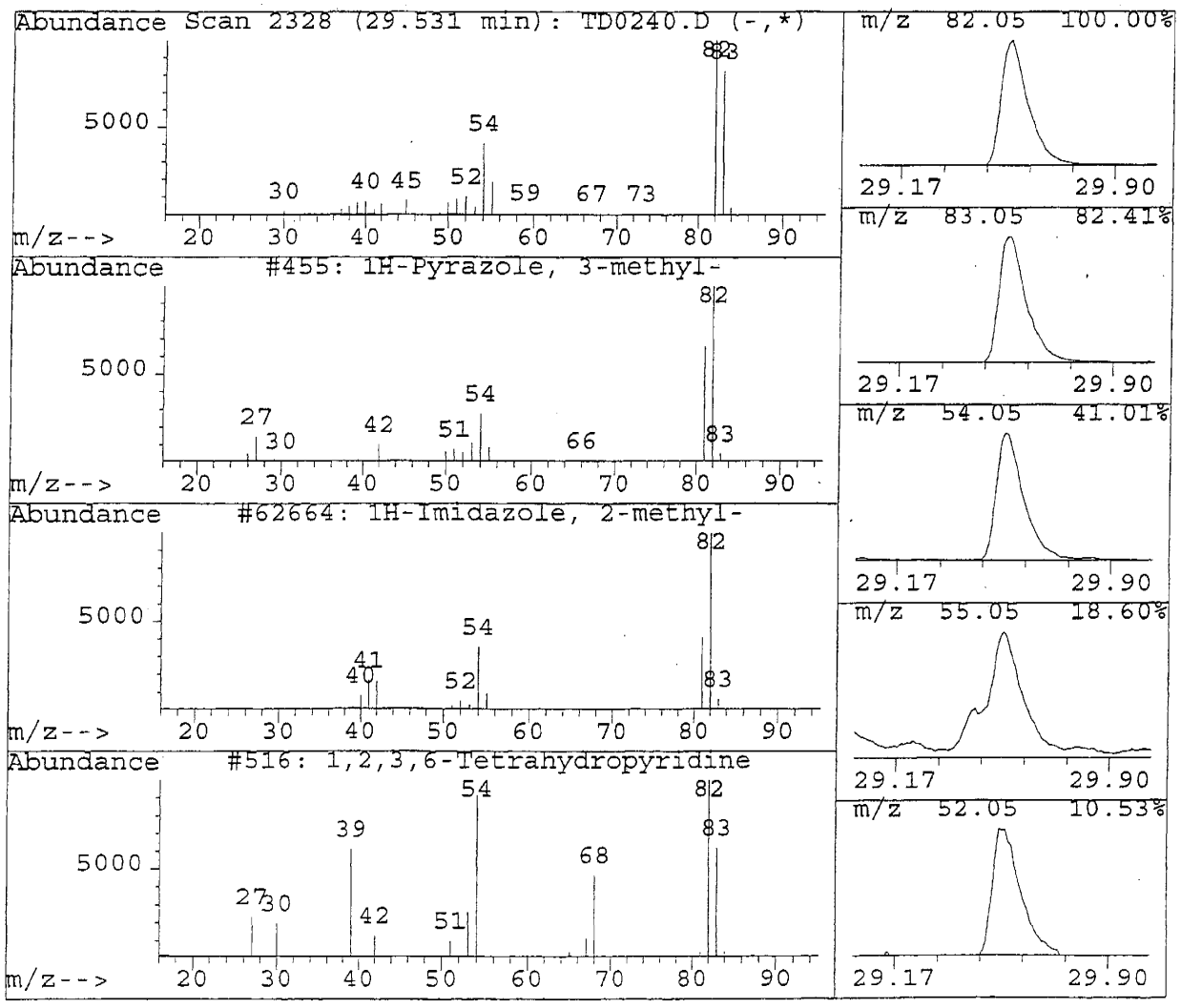
Library Search Compound Report

Data File : C:\HPCHEM\1\DATA\TODD\TD0240.D Vial: 1
Acq On : 17 Mar 95 2:09 pm Operator: J.T. SKEEN
Sample : TST#829 U-106 2.0L Inst : 5972 - In
Misc : SAMPLED 3/07/95 Multiplr: 1.00

Method : C:\HPCHEM\1\METHODS\TODD\HANFORD.M
Title : HANFORD TARGET ANALYTE - 5 POINT CALIBRATION
Library : C:\DATABASE\NBS75K.L

R.T.	Conc	Area	Relative to ISTD	R.T.
29.53	104.58 NG	1440948	BENZENE-D6	25.61

Hit# of 10	Tentative ID	Ref#	CAS#	Qual
1	1H-Pyrazole, 3-methyl-	455	001453-58-3	47
2	1H-Imidazole, 2-methyl-	62664	000693-98-1	47
3	1,2,3,6-Tetrahydropyridine	516	000694-05-3	42
4	Fomepizole	459	007554-65-6	17
5	2,6-Dimethyl-6-nitro-2-hepten-4-one	19157	073583-56-9	12



TD0240.D HANFORD.M Tue Mar 21 17:02:53 1995 HPPC Page 10