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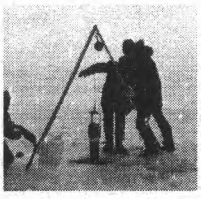
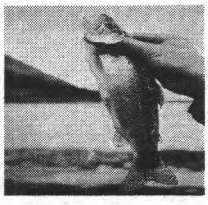
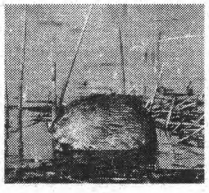
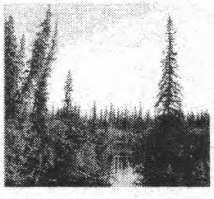
Northern River Basins Study



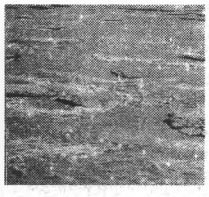



NORTHERN RIVER BASINS STUDY PROJECT REPORT NO. 111

BROAD SPECTRUM ANALYSIS OF MUNICIPAL AND INDUSTRIAL EFFLUENTS DISCHARGED INTO THE PEACE, ATHABASCA AND SLAVE RIVER BASINS: REVIEW OF GC-MS DATA, 1989 TO 1994 - VOLUME 1 OF 3



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by

C. Ian Johnson
Alberta Environmental Centre

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PREFACE:

The Northern River Basins Study was initiated through the "Canada-Alberta-Northwest Territories Agreement Respecting the Peace-Athabasca-Slave River Basin Study, Phase II - Technical Studies" which was signed September 27, 1991. The purpose of the Study is to understand and characterize the cumulative effects of development on the water and aquatic environment of the Study Area by coordinating with existing programs and undertaking appropriate new technical studies.

This publication reports the method and findings of particular work conducted as part of the Northern River Basins Study. As such, the work was governed by a specific terms of reference and is expected to contribute information about the Study Area within the context of the overall study as described by the Study Final Report. This report has been reviewed by the Study Science Advisory Committee in regards to scientific content and has been approved by the Study Board of Directors for public release.

It is explicit in the objectives of the Study to report the results of technical work regularly to the public. This objective is served by distributing project reports to an extensive network of libraries, agencies, organizations and interested individuals and by granting universal permission to reproduce the material.

This report contains referenced data obtained from sources external to the Northern River Basins Study. Individuals interested in using external data must obtain permission to do so from the donor agency.

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Whereas the above publication is the result of a project conducted under the Northern River Basins Study and the terms of reference for that project are deemed to be fulfilled,
IT IS THEREFORE REQUESTED BY THE STUDY OFFICE THAT;
this publication be subjected to proper and responsible review and be considered for release to the public.

F. J. Wrona — 14 May 96
(Dr. Fred J. Wrona, Science Director) (Date)

Whereas it is an explicit term of reference of the Science Advisory Committee "to review, for scientific content, material for publication by the Board",
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SUPPLEMENTAL COMMENTARY HAS BEEN ADDED TO THIS PUBLICATION: [ ] Yes [ ] No

R. Larkin — 2nd May 96
(Dr. P. A. Larkin, Ph.D., Chair) (Date)

Whereas the Study Board is satisfied that this publication has been reviewed for scientific content and for immediate health implications,
IT IS HERE APPROVED BY THE BOARD OF DIRECTORS THAT;
this publication be released to the public, and that this publication be designated for: **[ ] STANDARD AVAILABILITY [ ] EXPANDED AVAILABILITY**

Lucille Partington — May 29/96
(Lucille Partington, Co-chair) (Date)

Robert McLeod — May 21/96
(Robert McLeod, Co-chair) (Date)

BROAD SPECTRUM ANALYSIS OF MUNICIPAL AND INDUSTRIAL EFFLUENTS DISCHARGED INTO THE PEACE, ATHABASCA AND SLAVE RIVER BASINS: REVIEW OF GC-MS DATA, 1989 TO 1994

STUDY PERSPECTIVE

Under the Northern River Basins Study (NRBS), water, effluent, sediment and biota have been sampled extensively and analyzed for specific contaminants known to be associated with developments within the study area, or known to be transported by aerial transport. To date, only "target compound" contaminant analyses have been conducted on these samples, and the results show generally low levels of these compounds. However, these types of specific analyses do not include other potential contaminants that are not currently known to be associated with man-made developments within the basins, or aerial transport, or for which there is little understanding of their environmental effects. Target compound analyses have been done with selected ion monitoring gas chromatography or mass spectrometry (GC/MS) with specific detectors. However, this method gives no indication of the other non-target compounds present, nor does it provide an "archive" record of chromatograms. An alternative experimental approach to characterizing the major effluents and receiving waters of the Athabasca and Peace river systems is by broad spectrum analysis.

Related Study Questions

4a)	*What are the contents and nature of the contaminants entering the system and what is their distribution and toxicity in the aquatic ecosystem with particular reference to water, sediments and biota?*
8)	*Recognizing that people drink water and eat fish from these river systems, what is the current concentration of contaminants in water and edible fish tissue and how are these levels changing through time and by location?*
13b)	*What are the cumulative effects of man-made discharges on the water and aquatic environment?*

The project conducted broad spectrum analyses of water and effluent samples upstream and downstream of major effluent sources on the Athabasca, Peace and Wapiti-Smoky River systems. Analytical methods to classify organic constituents in effluents were based on full scan coupled GC/MS, and all significant compounds were characterized with respect to mass spectra and GC retention indices. The task was accomplished in three stages: (1) summary of results and review of raw GC/MS data from previous effluent analyses conducted between 1989 and 1994, (2) collection and analysis of current effluents, and (3) collection and analysis of receiving water samples.

Routine priority pollutant data for the analyses of municipal and industrial effluents, produced between 1989 and 1994, were reevaluated. Searchable mass spectral libraries were prepared for the organic components that were characterized. During that time period, improvements in effluent quality were observed, particularly for conventional bleached kraft mills. Generally, only low concentrations of contaminants were observed in sewage treatment plant (STP) effluent. Under the second task, 260 compounds were characterized from 1994 effluent samples, and a comparison of results revealed that the improvement in pulp mill effluent quality has continued. The third task determined that none of the contaminants observed in the discharged effluents were observed in surface waters in significant concentrations. Some of the compounds observed are ubiquitous in nature, and their presence cannot be attributed solely to industrial and municipal effluents.

Based on these results, it was concluded that the scope of future investigations should be narrowed to lipophilic classes of compounds in effluents and receiving waters, eliminating the compromises necessary to include hydrophilic compounds in the analysis. These analytical results will provide a permanent record of GC/MS data, allowing researchers to revisit the data in future years if other compounds become of interest.

This report provides a summary of the results and review of raw GC/MC data from previous effluent analysis conducted between 1989 and 1994 (Task 1). Information on the collection and analysis of current effluents (Task 2) is provided in Northern River Basins Study Project Report No. 121. Northern River Basins Study Project Report No. 138 provides analytical results arising from the collection and analysis of receiving water samples in 1994 (Task 3).

REPORT SUMMARY

Data produced at the Alberta Environmental Centre as part of the routine extractable priority pollutant GC-MS analysis of municipal and industrial effluents discharged into the northern Alberta river basins between 1989 and 1994 were reevaluated. The organic components of effluents were characterized by mass spectra and GC retention times and searchable mass spectral libraries were prepared. The improvement in effluent quality is demonstrated and discussed.

ACKNOWLEDGEMENTS

The authors gratefully to acknowledge the assistance of Grant Prill and Karen Hill of Alberta Envrionmental Centre for retrieving and compiling the GC-MS data, Brian Brownlee of National Water Research Institute for useful discussions and assistance in the preparation of this report and the Northern River Basins Study Board for partial funding of this work.

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1.0 INTRODUCTION

Under the Northern River Basins Study Board, water, effluent, sediment, fish and benthic invertebrates have been sampled extensively and analyzed for a wide variety of specific contaminants known to be associated with the developments within the northern basins. To date only target compound analysis for specific contaminants has been undertaken. These analyses are for specific contaminants and yield no information regarding other contaminants which may be present. To observe these other compounds full scan coupled gas chromatography-mass spectrometry (GC-MS) analysis of samples, followed by interpretation of the generated mass spectra is required.

Over the past decade, effluents and receiving waters in northern Alberta have been analyzed at the Alberta Environmental Centre (AEC) as part of numerous surveys and monitoring programs of Alberta Environmental Protection. Effluents and surface waters have been analyzed by GC-MS following the standard AEC Trace Organic Analysis Method A105.1 for extractable priority pollutants. This is a full scan method which yields spectra which can be used to identify or characterize the compounds present. These spectra can also be compiled to build searchable mass spectral libraries which can be used in future work.

This report describes the review of data produced in the analysis of effluents discharging into the Northern Basins during the period of 1989 to 1994. The impact of process changes implemented in kraft mills is also discussed. Futher, this report documents the methods by which spectra were obtained from the mass spectral data to produce the libraries.

2.0 MATERIALS AND METHODS

2.1 Acquisition of GC-MS Data

Effluent samples were collected and analyzed in accordance with AEC Method for Chemical Analysis of Trace Organics and Pesticides in Environmental Samples AECV92-M2. This method involves extraction of the effluent with methylene chloride at pH 10 and pH 2, and analyzing the concentrated, underivatized, combined extracts by GC-MS. GC-MS analysis was conducted using either a Hewlett Packard 5840 or a 5890 gas chromatograph eluting into a Hewlett Packard 5987 mass spectrograph operating in the EI/full scan mode. Data was collected

and stored with a Hewlett Packard RTE data system. Data was then converted to HP ChemStation G1034.C format for this project.

2.2 Analysis of GC-MS Results

GC-MS data was analyzed using HP Chemstation G1034.C software loaded on an ALR 486 computer. The Wiley mass spectral library was used as the reference library for probability bases matching (PBM) library searches. All spectra presented were "background subtracted". Background spectra for subtraction were obtained as the average of spectra over a 0.05 to 0.10 minute interval, in a region with no peak, near the peak under consideration.

Spectra of coeluting compounds were obtained by: i) identifying ions representation of each coeluting compounds (unique to the compound if possible, and as abundant as possible); ii) obtaining background subtracted spectra from the apex of peaks in the extracted ion chromatograms (EIC) for the ions representative of the compounds; and iii) for each compound, subtracting the component of the spectra from the other coeluting compounds (the amount determined from abundances in the EICs). An example is given in the Results and Discussion section.

2.3 Mass Spectral Evaluation and Library Compilation

Mass spectra were compared to the reference library using PBM software and evaluated using mass spectral interpretation techniques described by McLafferty (1980). Discussion of mass spectral interpretation is not presented in this report. In cases were retention indices were known, the order of elution of compounds was used as an aid in assigning structure. This was used extensively in the identification of mono-, sesqui-, and diterpenes. Mass spectra were stored in another PBM searchable reference library using HP Chemstation software. The system of cataloguing these spectra is described below.

The GC retention time of compounds was adjusted to standard retention times to facilitate comparison between chromatograms (retention times varied over the 5 years the data under consideration was obtained). Times were adjusted to one arbitrarily chosen chromatogram using

the slope and intercept obtained by regressing the retention times of 6 internal standards against the retention times in the reference chromatogram.

Effluent GC-MS chromatograms were divided in three groups: i) bleached kraft pulp mill effluents (BKME), ii) high yield pulp mill effluents which comprised both thermomechanical and chemi-thermomechanical pulp mill effluents (CTMP), and iii) municipal sewage treatment plant effluents (STP). Suncor effluent were considered separately. Separate searchable libraries were created for each group. Spectra are identified in the libraries by effluent type and the order in which there were considered. For example, BKME Peak 10, would be the 10th peak considered in the BKME chromatograms. These numbers are not necessarily in order of elution as spectra from several chromatograms were used to compile the libraries. Compounds were also named by elution order (using adjusted retention times) after the libraries were compiled. The performance of the libraries was evaluated using spectra from chromatograms not used to compile the libraries.

2.4 Quantitation of Compounds

Compounds were quantified using either d8-naphthalene or d12-benzo[a]anthracene as the internal standard. No standards for the compounds reported were run in the course of the analysis so compound concentrations were calculated assuming constant TIC response factors for compounds and internal standards. However, quantification was done by integrating EICs of ions representative of the compounds and standards. Representative ions were chosen on the basis of their uniqueness (to aid in compound identification and minimize interference of neighboring peaks) and the relative abundance in the compound mass spectrum. These ions are listed in Tables 1, 2, and 3. Relative response factors for the EIC signals were calculated as the ratio of proportion of abundance of the representative ion in the mass spectrum of the internal standard to the proportion of abundance of the representative ion in the mass spectrum of the compound. Compound relative response factors are also listed in Tables 1, 2, and 3. Effluent concentrations of compounds were calculated by dividing the EIC response of the compound by the EIC response of the internal standard, multiplying by the compound relative response factor and applying the analysis dilution factor.

3.0 RESULTS AND DISCUSSION

Compounds found in effluents are tabulated in Tables 1 (bleached kraft mill effluents), 2 (chemi-thermomechanical pulp mill effluents) and 3 (municipal sewage treatment plant effluents). The Suncor effluent is discussed separately. These compounds are characterized and described according to: i) tentative identification based on interpretation of mass spectra, mass spectral library search results, and elution order (evaluated using published retention indices) when ever possible, ii) Class/type of compound, i.e. chlorinated terpene, alkylated benzene, alkylated thiophene etc., iii) substructure such as carboxylic acid or incorporation of special elements such as chlorine or sulphur as determined from the molecular ion cluster, characteristic losses or characteristic ions.

The mass spectra of these conpounds attached to this report in Appendices 1, 2, and 3. They are also available in Probability Based Searchable digital format. Care must be used when using these spectra. They were obtained from complex chromatograms of unfractionated effluent extracts which required manipulation for most spectra. Figure 1 is a typical effluent chromatogram from which BKME spectra were obtained. Figure 2 shows a small region in which there are two peaks in the total ion chromatogram (TIC). Single ion chromatograms underneath the TIC indicate that there are at least 4 compounds eluted underneath these two TIC peaks. Spectra of these compounds were obtained by background subtraction, rescaling and subtraction of spectra of neighboring peaks. These manipulations can effect the low abundance ions in the spectra and limit the usefulness of the spectra for both structure elucidation and as a reference for PBM searching. However, with the additional chromatographic information, they should be useful in evaluating similar industrial effluents.

An important class of compounds identified in both CTMP effluents and BKME is the terpenoids, which are naturally produced compounds found in trees. This class of compounds can be subdivided into monoterpenes which contain 10 carbon atoms, sesquiterpenes which contain 15 carbon atoms, and diterpenes which contain 20 carbon atoms. Chlorinated derivatives of these compounds are also found in BKME.

Several monoterpenes were identified on the basis of their mass spectra and adjusted retention times. Identification could not be made on the basis of just one or the other. Mass spectra of monoterpenes are sufficiently similar to others of the class that identification solely on

the basis of the mass spectra, particularly when only low abundances of ions are present, is not possible (Laakso et. al. 1986). Kovats retention indices for monoterpenes on phases similar to those used in these analyses are reported in the literature (Davies 1990, Nykanen 1986). Kovats indices have been shown to be directly (linearly) related to the appearance temperatures of compounds eluting in temperature programmed gas chromatography (Watts and Kekwick 1974). It follows then that adjusted retention times should be linearly correlated with reported Kovats indices. A plot of Kovats indices and adjusted retention times is presented in Figure 3. There is a very strong correlation which illustrates the reliability with which the adjusted retention times may be used when evaluating data generated in the future. Unfortunately insufficient data is available in the literature to extend this analysis to other terpenoids.

Chlorinated terpenoids were also observed in BKME. The existence of these compounds has been previously reported by Stuthridge *et. al.* (1990). Mass spectra of the observed chlorinated monoterpenes in Alberta BKME were similar to those reported by Stuthridge *et. al.*

3.1 Bleached Kraft Mill Effluents

Four bleached kraft mills discharged effluent to the rivers in the Northern Basins between 1989 and 1994. Concentrations of contaminants observed in samples of these effluents are presented in Appendix 4 (the Weldwood mill in Hinton), Appendix 5 (the Procter and Gamble mill in Grande Prairie, recently purchased by Weyerhaeuser), Appendix 6 (the Daishowa mill in Peace River) and Appendix 7 (the AlPac mill in Grasslands). Only a hydrocarbon, identified as dimethylcyclohexane, dichloromethyl-methylsulphone and two diterpenes were detected in the AlPac effluent which employs nonconventional technology. This effluent will not be discussed further.

Compounds observed in the remaining three effluents can be divided into four broad groups:

1. Hydrocarbons, which include condensed products of polysaccharide hydrolysis produced during the cooking process; aromatic compounds resulting from the hydrolysis of lignin during the cooking process and nonylphenols observed in the effluent of the Weldwood mill, presumably added as a process chemical.

2. Terpenes, mono-, sesqui-, and di-, natural products in wood which are extracted in the cooking process.
3. Chlorinated compounds, resulting from the chlorination of compounds carried over from the cooking/pulping to the bleach plant or from the oxidative degradation/chlorination of residual lignin in the pulp during the chlorination plant.
4. Sulphur containing compounds produced during cooking process.

Summed concentrations of compounds of these types are presented, by mill, in Figures 4 to 15.

Process modifications implemented in these mills since 1989 have affected the character of the effluents. Better washing and oxygen delignification of pulp prior to bleaching reduce the organic material carried over to the bleach plant, resulting in dramatic decreases in hydrocarbon, terpenes and sulphur containing compounds in effluents. Replacement of chlorine with chlorine dioxide in the Hinton and Grande Prairie mills, and use of hydrogen peroxide in extraction stages, have resulted in large reductions in chlorinated terpenes and chlorinated aromatic compounds. Concentrations of 1,1-dichlorodimethylsulphone, also observed in the AlPac effluent are less affected. Similar effects are expected in the Peace River mill effluent where chlorine use has been eliminated since 1994.

3.2 Chemi-thermomechanical Pulp (CTMP) Mill Effluents

There were three CTMP mills operating in northern Alberta, discharging effluents to the northern river basins, during the 1989 to 1994 interval covered by this report. These comprise two in Whitecourt, operated by Millar Western and the Alberta Newsprint Company and one in Slave Lake operated by the Slave Lake Pulp Company. Similar processes were employed at all three mills but process details at individual mills differed. The exact nature of the differences are industry secrets and are not known. However, most differences in effluent quality between mills appear to be related to effluent treatment and not process technology. Compounds observed in effluents are shown in Table 2 and concentrations of these compounds are given, by mill, in Appendices 8 (Millar Western), 9 (Alberta Newsprint Company) and 10 (Slave Lake Pulp Company).

The CTMP process differs significantly from the kraft pulping process. In the kraft process lignin which holds individual fibers together is degraded and dissolved in hot caustic pulping liquors containing sodium sulphide. Wood chips and pulping liquors are discharged from the pulping vessel under great pressure (in the blow tank) where the chips are readily fiberized. The pulping liquors which contain the dissolved organic material, including the kraft lignin (that degraded and dissolved during the cooking process), and wood extractives such as the monoterpenoids are collected and returned to the chemical recovery system. Here the process chemicals are recovered and the organic material burned in the recovery system. The kraft cooking process is essentially a closed process with only chemicals lost as liquor carry-over to the bleach plant or lost in spills to the sewer, becoming part of the effluent. Most of the organic material in the effluent is produced in the bleach plant where residual lignin in the pulp is removed.

The CTMP process involves only the softening and not the removal of lignin from the pulp fibre. Wood chips, in which the lignin has been softened, are ground to fibre between two large, rotating plates. Neither chlorine bleaching nor sodium sulphide cooking are used in the process, so the chlorinated and sulphur containing compounds observed in BKME are not produced in CTMP mills. However, in Alberta CTMP mills there is no recovery system so that all the wood extractives dissolved in the pulping process enter the effluent stream.

Another significant difference between kraft and CTMP processes employed in Alberta is the species of woods used as feedstock. With the exception of AlPac, kraft mills use coniferous woods like lodge-pole pine while the CTMP mills use aspen. This results in considerable differences in the profile of extractives observed in effluents.

Effluent treatment processes also differ between pulping processes. Aerated sludge basins are sufficient to treat kraft mill effluents but the more concentrated CTMP effluents resulting from the lack of closure of the pulping process have to be treated in high rate activated sludge basins. Effluent analyses reviewed for this report suggest that these treatment process are prone to breakdown, resulting in episodes of discharge of concentrated effluent.

The compounds observed in CTMP effluents can be separated into two groups:

1. Wood natural products such as terpenoids, naturally produced aromatic compounds and naturally produced organic acids.

2. Anthropogenic compounds, principally phthalates.

Very little organic material was observed in Alberta Newsprint Company mill effluents. Figures 16 to 19 show the level of the above compounds in Millar Western and Slave Lake Pulp mill company effluents. The episodic nature of discharge concentrations and a large overall reduction over time is illustrated.

In addition several anthropogenic compounds have been observed in the Slave Lake Pulp Company mill effluents in high concentrations. These compounds are not generally associated with the CTMP process and we can give no reason for their presence in the effluent. However, because of the high concentration of these compounds we are quite confident of the identifications. These compounds and the concentrations observed in effluents are shown in Table 4. The toxicities of some of these compounds suggest that there may be environmental effects.

3.3 Municipal Sewage Treatment Plant (STP) Effluents

Concentrations of contaminants observed in STP effluents are listed in Appendix 11. Most are present only in low concentrations (<1.0 µg/L) and would not be expected to be observed in river waters after dilution. Notable exceptions are caffeine, some phosphates and some phthalates. Even these are usually present in concentrations less than 10 µg/L. No decreasing or increasing trends over time are obvious in the data. There are differences in the composition of effluents. Caffeine is present in high concentrations in Athabasca and Fort McMurray effluents but not present in the Whitecourt effluents and in lower concentrations in the Grande Prairie effluents. The other major contaminants are 2-butoxyethyl phosphate in the Fort McMurray and Athabasca effluents, tributylphosphate in the Grande Prairie effluent, and bis(ethylhexyl)phthalate in the Whitecourt and Fort McMurray effluents.

3.4 Suncor Process Effluent

Total ion chromatograms of extracts of the Suncor process effluent are shown in Figure 20. The only GC peaks are internal and surrogate standards added in amounts correlating to

10 µg/L in the effluent. The large unresolved "hump" in the 1992 chromatogram is hydrocarbons, probably naphthenic acids and other hydrocarbons which they solubilize in aqueous solution. Given the uncertainty of the nature of this material it is not possible to produce reliable estimates of contamination. It is obvious that a dramatic reduction has occurred during the period between the 1992 and the 1993 times of sampling.

4.0 SUMMARY

Great improvements in the effluent quality of conventional kraft mills operating before 1989 were observed over the review period. This is the result of process changes and treatment improvements implemented during the review period. Only very low concentrations of contaminants were observed in the effluent of the AlPac mill which began operating in the fall of 1993.

Episodes of high concentrations of contaminants were observed in two of the three CTMP mills. These were likely due to problems in the treatment system. Such episodes were not observed in the Alberta Newsprint Company effluent. In addition to the expected natural products, high concentrations of chemicals not generally associated with the CTMP process were observed in the Slave Lake Pulp effluent.

Generally only low concentrations of contaminants were observed in STP effluents. Major contaminants observed were caffeine, phosphates and phthalates.

Contaminants in the Suncor process effluent could not be resolved by GC but mass spectra indicated that they were hydrocarbon in nature. A large decrease in this material was observed in between the 1992 and 1993 samples.

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Table 1. Compounds in kraft mill effluents.

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 001	Peak 123	Dimethylsulphoxide (86)	5.18	78	0.549
Cmpd 002	Peak 1	Methylcyclohexane	6.15	112	0.111
Cmpd 003	Peak 124	2-Heptanone (91)	6.25	58	0.333
Cmpd 004	Peak 1a	Dimethylcyclohexane	6.26	112	0.112
Cmpd 005	Peak 125	$C_7H_{12}O$	6.38	98	0.178
Cmpd 006	Peak 2	$C_4H_6S_2$	6.44	75	0.274
Cmpd 007	Peak 3	Methylcyclopentenone	6.72	96	0.184
Cmpd 008	Peak 126	Ethanone, 1-(2-furanyl) (72) Likely contains sulphur	6.78	95	0.500
Cmpd 009	Peak 4	Dimethylsulphone	7.25	79	0.382
Cmpd 010	Peak 5	Diethylcyclopentenone	7.53	110	0.126
Cmpd 011	Peak 127	Methylcyclopentenone	8.18	96	0.332
Cmpd 012	Peak 6	Dimethyltrisulphide	8.33	126	0.202
Cmpd 013	Peak 7	Diethylcyclopentenone	8.94	95	0.354
Cmpd 014	Peak 8	α-Phellandrene (91)	9.19	93	0.257
Cmpd 015	Peak 9	Monoterpene [1] ($C_{10}H_{16}O$)	9.34	93	0.102
Cmpd 016	Peak 10	Unidentified	9.40	81	0.151
Cmpd 017	Peak 11	α-Terpinene (96)	9.52	121	0.150
Cmpd 018	Peak 12	*p*-Cymene (91)	9.77	119	0.214
Cmpd 019	Peak 13	Guaiacol 80	9.77	124	0.175
Cmpd 020	Peak 14	1,2-bis(methylthio)ethane	9.82	122	0.143
Cmpd 021	Peak 15	β-Phellandrene (87)	9.88	93	0.222
Cmpd 022	Peak 16	Unidentified	9.95	96	0.216
Cmpd 023	Peak 17	Dimethylcyclopentenone	10.16	110	0.240
Cmpd 024	Peak 18	1,3-Dichlorodimethylsulphone	10.28	113	0.101
Cmpd 025	Peak 91	3,5-Dimethylcyclopentane-1,2-dione (64)	10.50	126	0.153
Cmpd 026	Peak 19	Guaiacol 76 (spectrum very similar to Cmpd 019)	10.84	109	0.196
Cmpd 027	Peak 20	1-phenylethanone (94)	10.93	105	0.219
Cmpd 028	Peak 21	Monoterpene	11.05	99	0.091
Cmpd 029	Peak 22	1-(2-thienyl)ethanone (86)	11.36	111	0.268
Cmpd 030	Peak 24	1-methyl-4-(1-methylethenyl)benzene (92)	11.49	132	0.110
Cmpd 031	Peak 25	1-(2-thienyl)ethanone	11.58	111	0.337
Cmpd 032	Peak 140	Fenchone (83)	11.60	81	0.332
Cmpd 033	Peak 129	Thioanisole	11.61	109	0.331

Table 1. Compounds in kraft mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 034	Peak 26	Unidentified Hydrocarbon	11.74	140	0.122
Cmpd 035	Peak 27	Unidentified (contains sulphur)	11.81	124	0.110
Cmpd 036	Peak 28	Unidentified (contains sulphur)	11.86	123	0.244
Cmpd 037	Peak 29	Hydrocarbon (see binder)	11.89	125	0.108
Cmpd 038	Peak 30	{Methylguaiacol 80}	12.00	123	0.215
Cmpd 039	Peak 31	1,1-Dichlorodimethylsulphone	12.33	83	0.335
Cmpd 040	Peak 32	Methyl (methylthio)methyl disulphide	12.53	140	0.061
Cmpd 041	Peak 137	Terpenone	12.81	109	0.097
Cmpd 042	Peak 33	Unidentified hydrocarbon	12.86	83	0.083
Cmpd 043	Peak 34	{Veratrole 96}	12.99	138	0.105
Cmpd 044	Peak 35	C7H8O3 (based on MI)	13.09	140	0.063
Cmpd 045	Peak 138	Camphor (96)	13.10	95	0.149
Cmpd 046	Peak 92*	Unidentified	13.12	94	0.188
Cmpd 047	Peak 36	Alkylated cyclopentenone	13.16	138	0.089
Cmpd 048	Peak 37	Unidentified	13.22	140	0.030
Cmpd 049	Peak 38	Unidentified	13.42	138	0.085
Cmpd 050	Peak 39	Unidentified	13.47	140	0.041
Cmpd 051	Peak 40	1-Phenylpropanone (90)	13.55	105	0.327
Cmpd 052	Peak 41	Monoterpene(s)	13.60	97	0.049
Cmpd 053	Peak 42	Unidentified	13.68	126	0.081
Cmpd 054	Peak 44	Dichlorophenol	13.88	162	0.129
Cmpd 055	Peak 130*	Methylphenylsulphone	14.08	125	0.258
Cmpd 056	Peak 46	2-(2-Thienyl)propanal	14.08	111	0.479
Cmpd 057	Peak 47	t-Butylthiophene	14.13	125	0.392
Cmpd 058	Peak 48a	Coeluting Monoterpene and alkylcyclohexenone	14.15	125	0.094
Cmpd 059	Peak 48b	Coeluting Monoterpene and alkylcyclohexenone	14.15	123	0.043
Cmpd 060	Peak 111	Benzenemethanol, 4-(1-methylethyl) (59)	14.37	135	0.223
Cmpd 061	Peak 49	Coeluting Monoterpenes	14.51	95	0.061
Cmpd 062	Peak 50	4-Methylthiophenol	14.58	125	0.272
Cmpd 063	Peak 51	Coeluting monoterpenes	14.61	107	0.142
Cmpd 064	Peak 52	Dimethyltetrasulphide	14.91	158	0.070
Cmpd 065	Peak 53	Monoterpenone	14.99	137	0.469
Cmpd 066	Peak 131	Contains dichloromethyl	15.53	83	0.304

Table 1. Compounds in kraft mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 067	Peak 113	Contains Sulphur S4	16.51	164	0.137
Cmpd 068	Peak 112	3-methyl-2-thiophenecarboxylic acid (53)	16.61	142	0.133
Cmpd 069	Peak 132	not identified	17.09	110	0.259
Cmpd 070	Peak 54	Coeluting Compounds; 1 is monoterpene.	17.30	135	0.079
Cmpd 071	Peak 55	methyl(1-methylethyl)phenol (62)	17.51	135	0.156
Cmpd 072	Peak 56	Monoterpene	17.56	152	0.081
Cmpd 073	Peak 57	Unidentified	17.83	125	0.024
Cmpd 074	Peak 58	Mulitple Compounds (Monoterpenes)	18.21	109	0.102
Cmpd 075	Peak 133	Syringol (94)	18.25	154	0.224
Cmpd 076	Peak 134	Chloroterpene	18.31	87	0.211
Cmpd 077	Peak 59b	Monoterpene	18.49	95	0.056
Cmpd 078	Peak 59c	Trichlorophenol	18.55	196	0.225
Cmpd 079	Peak 93	Alkylnaphthalene	18.85	141	0.181
Cmpd 080	Peak 94	Vanillin (74)	19.46	152	0.133
Cmpd 081	Peak 135, 60a, and 114	Junipene (83)	19.56	161	0.041
Cmpd 082	Peak 60b	Alkylbenzene	19.58	91	0.368
Cmpd 083	Peak 60c	Dimethoxybenzoic acid (25)	19.61	182	0.120
Cmpd 084	Peak 61	Chlorinated monoterpene ??	19.66	187	0.076
Cmpd 085	Peak 95	Monoterpene	20.41	119	0.132
Cmpd 086	Peak 62	Coeluting compounds Terpenoid	20.47	93	0.148
Cmpd 087	Peak 96	Monoterpene	20.51	135	0.136
Cmpd 088	Peak 97	Chloromonoterpene	20.56	164	0.109
Cmpd 089	Peak 98	Methoxy-2-ethoxyethyl-1-furan (53)	20.64	97	0.375
Cmpd 090	Peak 63	Dichloro- Methyl terpenoid	21.26	196	0.054
Cmpd 091	Peak 64	Dichloroguaiacol	21.36	177	0.074
Cmpd 092	Peak 99	Acetovanillone	21.42	151	0.215
Cmpd 093	Peak 65	Alkylthiophene	21.48	139	0.232
Cmpd 094	Peak 66	Trichloroveratrole	21.74	206	0.079
Cmpd 095	Peak 115	(+)-Aromadendrene (78)	21.83	161	0.048
Cmpd 096	Peak 116	d-Cadinene (64)	21.98	161	0.084
Cmpd 097	Peak 67a	Sesquiterpene (204), not Peak 116	21.99	204	0.056
Cmpd 098	Peak 67b	Dichloro compounds 221,223,225 no MI.	21.99	221	0.033

Table 1. Compounds in kraft mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 099	Peak 117	Sesquiterpene mw 202	22.03	159	0.152
Cmpd 100	Peak 100	Sesquiterpene	22.13	161	0.065
Cmpd 101	Peak 101	Unknown (terpenoid)	22.23	124	0.119
Cmpd 102	Peak 68	Dichloro, methyl loss,terpenoid	22.52	203	0.079
Cmpd 103	Peak 69	Sesquiterpene C14H24O	22.63	138	0.081
Cmpd 104	Peak 70	Dichloro compounds 221,223,225 no MI., terpenoid	22.70	221	0.090
Cmpd 105	Peak 136	Ethanone, 1-(3,4-Dimethoxyphenyl) (86)	22.81	165	0.230
Cmpd 106	Peak 71	Chlorovanillone	22.88	186	0.100
Cmpd 107	Peak 72	Dichloro, terpenoid	23.08	203	0.052
Cmpd 108	Peak 73	Unidentified chlorinated hydrocarbon	23.16	109	0.090
Cmpd 109	Peak 118	Trichloroguaiacol	23.64	211	0.182
Cmpd 110	Peak 74	Terpenoid	23.64	153	0.061
Cmpd 111	Peak 102	coeluting compounds	24.21	142	0.066
Cmpd 112	Peak 75	Unidentified hydrocarbons	24.54	156	0.057
Cmpd 113	Peak 76	Trichlorinated terpene	25.04	179	0.050
Cmpd 114	Peak 77	Unidentified, contains S	25.32	176	0.087
Cmpd 115	Nonylphenol Isomer [1]	Nonylphenol Isomer [1]	25.76	121	0.161
Cmpd 116	Nonylphenol Isomer [2]	Nonylphenol Isomer [2]	25.92	135	0.445
Cmpd 117	Nonylphenol Isomer [3]	Nonylphenol Isomer [3]	26.08	135	0.184
Cmpd 118	Nonylphenol Isomer [4]	Nonylphenol Isomer [4]	26.18	149	0.170
Cmpd 119	Nonylphenol Isomer [5]	Nonylphenol Isomer [5]	26.24	135	0.288
Cmpd 120	Nonylphenol Isomer [6]	Nonylphenol Isomer [6]	26.29	149	0.181
Cmpd 121	Nonylphenol Isomer [7]	Nonylphenol Isomer [7]	26.50	135	0.240
Cmpd 122	Peak 78	3,4,5-Trimethoxybenzaldehyde (50)	26.54	196	0.250
Cmpd 123	Nonylphenol Isomer [8]	Nonylphenol Isomer [8]	26.57	121	0.145
Cmpd 124	Nonylphenol Isomer [9]	Nonylphenol Isomer [9]	26.65	149	0.191
Cmpd 125	Nonylphenol Isomer [10]	Nonylphenol Isomer [10]	26.73	135	0.187
Cmpd 126	Nonylphenol Isomer [11]	Nonylphenol Isomer [11]	26.81	135	0.438
Cmpd 127	Nonylphenol Isomer [12]	Nonylphenol Isomer [12]	26.99	149	0.281
Cmpd 128	Peak 119	Diterpenoid (nor)	28.87	243	0.049
Cmpd 129	Peak 120	Diterpene	29.40	241	0.036

Table 1. Compounds in kraft mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 130	Peak 121	Diterpene	29.56	123	0.225
Cmpd 131	Peak 122	Diterpene	29.68	137	0.104
Cmpd 132	Peak 104	Diterpene	30.00	93	0.053
Cmpd 133	Peak 80	Sandaracopimaradiene	30.29	137	0.067
Cmpd 134	Peak 81	Diterpene	31.10	109	0.045
Cmpd 135	Peak 105	Diterpene	31.45	159	0.042
Cmpd 136	Peak 106	Diterpene	31.66	137	0.051
Cmpd 137	Peak 82	Diterpene	32.07	255	0.057
Cmpd 138	Peak 141	Diterpene	32.13	137	0.041
Cmpd 139	Peak 107	Diterpene	32.32	232	0.033
Cmpd 140	Peak 83	Diterpene	32.53	229	0.032
Cmpd 141	Peak 143	8,12.XI.-Epoxylabd-14-en-13.XCI.-ol unide	32.97	191	0.131
Cmpd 142	Peak 142	(11E,13Z)-11813-Labdadien-8-ol (59)	33.13	177	0.081
Cmpd 143	Peak 144	(11E,13Z)-11813-Labdadien-8-ol (55)	33.72	177	0.067
Cmpd 144	Peak 86	Pimarinal	33.93	257	0.026
Cmpd 145	Peak 145	4-Androsten-3-one (22)	34.21	239	0.083
Cmpd 146	Peak 108	Diterpene	34.79	187	0.035
Cmpd 147	Peak 109	Diterpene	36.03	259	0.121
Cmpd 148	Peak 110	Diterpene	36.18	137	0.128
Cmpd 149	Peak 89	Coeluting compounds	38.63	185	0.051

Table 2. Compounds in CTMP mill effluents.

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 001	CTMP Peak 21	Hexanal	4.14	82	0.0471
Cmpd 002	CTMP Peak 22	3-Methylbutanoic Acid	5.40	60	0.5448
Cmpd 003	CTMP Peak 23	2-Methylbutanoic Acid	5.60	74	0.4329
Cmpd 004	CTMP Peak 28	Pentanoic Acid	6.16	60	0.5005
Cmpd 005	CTMP Peak 29	Cyclohexanone	6.36	98	0.1658
Cmpd 006	CTMP Peak 24	Monoterpene (α-Thujene)	7.17	93	0.2861
Cmpd 007	CTMP Peak 1	Benzaldehyde	8.11	105	0.2174
Cmpd 008	CTMP Peak 25	Monoterpene (Sabinene)	8.42	93	0.2652
Cmpd 009	CTMP Peak 26	Hexanoic Acid	8.57	60	0.4009
Cmpd 010	CTMP Peak 27	1-(Methylethenyl)-benzene	8.63	118	0.2141
Cmpd 011	CTMP Peak 30	Monoterpene (α-Phellandrene)	9.24	93	0.3288
Cmpd 012	CTMP Peak 31	Monoterpene (α-Terpinene)	9.56	121	0.1909
Cmpd 013	CTMP Peak 32	Monoterpene (*p*-Cymene)	9.78	119	0.4048
Cmpd 014	CTMP Peak 87	2,2'-Azobis[2-methylpropanenitrile]	9.86	69	0.4437
Cmpd 015	CTMP Peak 33	Monoterpene (β-Thujene)	9.92	93	0.3348
Cmpd 016	CTMP Peak 34	Monoterpene (γ-Terpinene)	10.69	93	0.2590
Cmpd 017	CTMP Peak 35	Monoterpene	11.49	136	0.1216
Cmpd 018	CTMP Peak 86	4-Methylphenol	11.51	107	0.1861
Cmpd 019	CTMP Peak 69	Monoterpene	11.53	132	0.0178
Cmpd 020	CTMP Peak 36	α,α-Dimethylbenzenemethanol	11.63	121	0.2669
Cmpd 021	CTMP Peak 88	Unidentified Amine	12.45	115	0.2378
Cmpd 022	CTMP Peak 4	C8 Acid (C8H16O2)	12.49	88	0.2841
Cmpd 023	CTMP Peak 13	Monoterpene	12.77	109	0.0806
Cmpd 024	CTMP Peak 37	Monoterpene	12.96	83	0.2180
Cmpd 025	CTMP Peak 38	Unidentified Hydrocarbon	13.23	87	0.1964
Cmpd 026	CTMP Peak 39	Alkylbenzene	13.29	91	0.2197
Cmpd 027	CTMP Peak 40	Benzoic Acid	13.39	122	0.2197

Table 2. Compounds in CTMP mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 028	CTMP Peak 41	Octanoic Acid	13.59	60	0.2090
Cmpd 029	CTMP Peak 14	4-(1-methylethyl)-benzenemethanol	14.07	135	0.1626
Cmpd 030	CTMP Peak 42	Monoterpene	14.11	96	0.1471
Cmpd 031	CTMP Peak 15	Terpinol	14.19	93	0.1116
Cmpd 032	CTMP Peak 43	Monoterpene	14.26	81	0.0970
Cmpd 033	CTMP Peak 106	Monoterpene	14.38	107	0.1170
Cmpd 034	CTMP Peak 44	Hydrocarbon	15.00	116	0.1770
Cmpd 035	CTMP Peak 17	Benzothiazole	15.06	135	0.4507
Cmpd 036	CTMP Peak 45	Benzeneacetic Acid	15.85	91	0.5041
Cmpd 037	CTMP Peak 5	OXY Hydrocarbon	15.83	57	0.2312
Cmpd 038	CTMP Peak 16	Hydrocarbon	16.34	67	0.1405
Cmpd 039	CTMP Peak 107	Methylnaphthalene	16.48	142	0.2674
Cmpd 040	CTMP Peak 46	Indole	16.77	117	0.3793
Cmpd 041	CTMP Peak 108	Methylnaphthalene	16.90	142	0.2840
Cmpd 042	CTMP Peak 18	Monoterpene	17.20	150	0.1552
Cmpd 043	CTMP Peak 120	Alkyl Phenol	18.20	107	0.3740
Cmpd 044	CTMP Peak 47	Monoterpene	18.26	79	0.1933
Cmpd 045	CTMP Peak 6	OXY Hydrocarbon	18.27	87	0.2191
Cmpd 046	CTMP Peak 48	Decanoic Acid	18.33	60	0.2059
Cmpd 047	CTMP Peak 49	Sesquiterpene	18.59	161	0.0536
Cmpd 048	CTMP Peak 8	Oxyhydrocarbon	18.60	57	0.3058
Cmpd 049	CTMP Peak 7	OXY Hydrocarbon	18.67	57	0.3045
Cmpd 050	CTMP Peak 89	Unidentified Hydrocarbon	18.96	124	0.1168
Cmpd 051	CTMP Peak 2	Vanillin	19.27	151	0.2397
Cmpd 052	CTMP Peak 90	Unidentified Amine	20.83	128	0.1447
Cmpd 053	CTMP Peak 50	Pentadecane	21.18	57	0.2094
Cmpd 054	CTMP Peak 91	Acetovanillone	21.34	151	0.2922
Cmpd 055	CTMP Peak 8	Monterpene	21.36	110	0.1806

Table 2. Compounds in CTMP mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 056	CTMP Peak 64	Monoterpene Acetate ??	21.88	180	0.0682
Cmpd 057	CTMP Peak 64	Unidentified	22.00	180	0.0859
Cmpd 058	CTMP Peak 92	Unidentified	22.63	178	0.0944
Cmpd 059	CTMP Peak 51	Monoterpene	22.76	168	0.0840
Cmpd 060	CTMP Peak 55a	Syringaldehyde	23.01	182	0.3119
Cmpd 061	CTMP Peak 51	Monoterpene Acid	23.11	168	0.1112
Cmpd 062	CTMP Peak 52	Hexadecane	23.25	57	0.2258
Cmpd 063	CTMP Peak 53	Unidentified Hydrocarbon	23.58	127	0.0442
Cmpd 064	CTMP Peak 19	2-(Methylthio)benzothiazole	23.66	181	0.1869
Cmpd 065	CTMP Peak 109	Diphenylamine	23.68	169	0.2410
Cmpd 066	CTMP Peak 3	Sesquiterpene	23.95	133	0.2642
Cmpd 067	CTMP Peak 70	Unidentified	24.30	147	0.2755
Cmpd 068	CTMP Peak 54	Unidentified Hydrocarbon	24.41	157	0.0748
Cmpd 069	CTMP Peak 71	Unidentified	24.61	126	0.0939
Cmpd 070	CTMP Peak 9	1,3,5-tri-2-propenyl-1,3,5-triazine-2,4,6(1H,3H,5H)-trione	24.73	249	0.1367
Cmpd 071	CTMP Peak 55b	Heptadecene	24.83	69	0.0819
Cmpd 072	CTMP Peak 56	Heptadecene	24.91	69	0.0983
Cmpd 073	CTMP Peak 72	Sesquiterpene	24.95	202	0.0816
Cmpd 074	CTMP Peak 57	Heptacecane	25.23	57	0.2196
Cmpd 075	CTMP Peak 121	Cyclododecane of Dodecene	25.39	55	0.1987
Cmpd 076	CTMP Peak 10	Monoterpene	25.62	83	0.2571
Cmpd 077	CTMP Peak 73	Sequiterpene	25.74	202	0.0942
Cmpd 078	CTMP Peak 74	Sesquiterpene	26.05	189	0.1727
Cmpd 079	CTMP Peak 94	Syringone	26.35	181	0.1978
Cmpd 080	CTMP Peak 58	Methylheptadecane	26.39	57	0.1930
Cmpd 081	CTMP Peak 59	Hydrocarbon	27.42	110	0.2260
Cmpd 082	CTMP Peak 112	N-Butyl-benzenesulphonamide	27.43	170	0.2271

Table 2. Compounds in CTMP mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 083	CTMP Peak 122	OXYhydrocarbon	27.77	69	0.4693
Cmpd 084	CTMP Peak 60	Diterpene	29.32	241	0.0384
Cmpd 085	CTMP Peak 75	Sesquiterpene	29.36	185	0.1953
Cmpd 086	CTMP Peak 95	Sesquiterpene	29.53	165	0.0457
Cmpd 087	CTMP Peak 96	Unidentified	30.08	205	0.1286
Cmpd 088	CTMP Peak 11	Dibutylphthalate	30.09	149	0.5754
Cmpd 089	CTMP Peak 61	Diterpene (Sandaracopimaradiene)	30.22	137	0.1057
Cmpd 090	CTMP Peak 113	N-Phenylbenzamide	30.37	105	0.4271
Cmpd 091	CTMP Peak 123	Hexadecanoic Acid	30.53	129	0.0430
Cmpd 092	CTMP Peak 97	Sesquiterpene	30.62	232	0.0523
Cmpd 093	CTMP Peak 124	Sesquiterpene	30.94	205	0.0896
Cmpd 094	CTMP Peak 62	Diterpene	31.03	257	0.0252
Cmpd 095	CTMP Peak 119	Sulphur S8	31.69	256	0.1183
Cmpd 096	CTMP Peak 98	Sesquiterpene	31.72	137	0.2637
Cmpd 097	CTMP Peak 63	Diterpene	32.43	272	0.0373
Cmpd 098	CTMP Peak 125	Linoleic Acid	33.35	67	0.1111
Cmpd 099	CTMP Peak 99	Unidentified	34.37	246	0.0544
Cmpd 100	CTMP Peak 114	Unidentified	34.59	264	0.0374
Cmpd 101	CTMP Peak 115	Unidentified	35.52	150	0.0667
Cmpd 102	CTMP Peak 100	Unidentified	35.76	229	0.1681
Cmpd 103	CTMP Peak 76	Diterpene	35.87	150	0.0719
Cmpd 104	CTMP Peak 101	Diterpene	36.08	135	0.0687
Cmpd 105	CTMP Peak 12	Bis(2-ethylhexyl)phthalate	38.82	149	0.3556
Cmpd 106	CTMP Peak 102	Diterpene	40.29	159	0.1197
Cmpd 107	CTMP Peak 77	Squalene	42.35	69	0.2599
Cmpd 108	CTMP Peak 65	Triterpene	44.06	365	0.0391
Cmpd 109	CTMP Peak 78	Triterpene	44.43	396	0.0133
Cmpd 110	CTMP Peak 79	Triterpene	46.17	394	0.0221

Table 2. Compounds in CTMP mill effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 111	CTMP Peak 66	Triterpene	46.37	396	0.0268
Cmpd 112	CTMP Peak 20	Sterol	46.40	386	0.0141
Cmpd 113	CTMP Peak 80	Triterpene	46.61	396	0.0226
Cmpd 114	CTMP Peak 81	Triterpene	49.03	409	0.0161
Cmpd 115	CTMP Peak 82	Triterpene	49.65	414	0.0216
Cmpd 116	CTMP Peak 83	Triterpene	50.38	411	0.0772
Cmpd 117	CTMP Peak 67	Triterpene	50.70	409	0.0233
Cmpd 118	CTMP Peak 84	Triterpene	51.27	218	0.0712
Cmpd 119	CTMP Peak 68	Triterpene	52.15	218	0.0680

Table 3. Compounds in municipal STP effluents.

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 01	STP Peak 58	Alkylfuran	5.07	108	0.298
Cmpd 02	STP Peak 51	Cyclohexanol	6.14	82	0.217
Cmpd 03	STP Peak 33	Dichlorinated Hydrocarbon	6.75	103	0.105
Cmpd 04	STP Peak 34	C7 Amine (Tertiary)	6.95	115	0.065
Cmpd 05	STP Peak 35	Sulphonylbismethane	7.01	94	0.265
Cmpd 06	STP Peak 21	Cyclohexanone	7.07	98	0.162
Cmpd 07	STP Peak 22	Trichloropropane	7.26	110	0.099
Cmpd 08	STP Peak 76	Alkene (C12)	8.95	57	0.474
Cmpd 09	STP Peak 77	Alkene (C12)	9.21	97	0.259
Cmpd 10	STP Peak 36	Isocineole	9.50	111	0.131
Cmpd 11	STP Peak 37	OXY Hydrocarbon	9.54	101	0.146
Cmpd 12	STP Peak 23	Dichlorobenzene	9.55	146	0.222
Cmpd 13	STP Peak 38	Alkyl Benzene	9.70	105	0.356
Cmpd 14	STP Peak 59	OXY Hydrocarbon	9.82	103	0.092
Cmpd 15	STP Peak 79	Alkylbenzene	10.88	105	0.297
Cmpd 16	STP Peak 24	Nitrosomorpholine	11.14	116	0.172
Cmpd 17	STP Peak 80	Alkylbenzene	11.95	119	0.318
Cmpd 18	STP Peak 1	1,1-Dichlorodimethylsulphone	12.09	83	0.282
Cmpd 19	STP Peak 88	Alkylbenzene	12.19	119	0.466
Cmpd 20	STP Peak 25	Unidentified Alkoxy compound	12.25	73	0.078
Cmpd 21	STP Peak 81	Alkylbenzene	12.30	119	0.484
Cmpd 22	STP Peak 52	Triethylphosphate	12.43	155	0.194
Cmpd 23	STP Peak 2	Unidentified Amine (Morpholine)	12.46	115	0.118
Cmpd 24	STP Peak 26	Decamethylcyclopentasiloxane	13.07	267	0.117
Cmpd 25	STP Peak 39	Monoterpene ($C_{10}H_{16}O$)	13.15	119	0.296
Cmpd 26	STP Peak 3	2-Ethylcyclohexanone	13.60	140	0.051
Cmpd 27	STP Peak 27	Unidentified Monochloroamine	14.15	134	0.073

Table 3. Compounds in municipal STP effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 28	STP Peak 60	Unidentified hydrocarbon	14.16	119	0.099
Cmpd 29	STP Peak 4b	*t*-Butylcyclohexanone	15.11	98	0.256
Cmpd 30	STP Peak 4a	1,2-Benzothiazole	15.13	135	0.296
Cmpd 31	STP Peak 40	Terpenol	15.56	139	0.056
Cmpd 32	STP Peak 41	Chlorinated amine	15.93	133	0.188
Cmpd 33	STP Peak 82	Unidentified alkene	15.93	112	0.151
Cmpd 34	STP Peak 42	Unidentified	15.99	97	0.119
Cmpd 35	STP Peak 43a	Alkyl Indene	16.32	129	0.088
Cmpd 36	STP Peak 43b	Terpene	16.35	108	0.090
Cmpd 37	STP Peak 83	Alkylbenzene	16.41	133	0.192
Cmpd 38	STP Peak 29	Alkyl Indanone	16.52	131	0.142
Cmpd 39	STP Peak 28	Dimethyl phenol	16.78	122	0.148
Cmpd 40	STP Peak 44	Alkyl Indan	16.79	145	0.099
Cmpd 41	STP Peak 30	Monoterpene	17.02	152	0.054
Cmpd 42	STP Peak 84	Branched alkene	17.25	97	0.226
Cmpd 43	STP Peak 31	Unidentified chlorinated compound	17.30	133	0.096
Cmpd 44	STP Peak 5b	Unidentified	17.30	341	0.024
Cmpd 45	STP Peak 5a	Propenyl Anisole	17.33	148	0.064
Cmpd 46	STP Peak 53	1,3-Isobenzofurandione	17.36	104	0.307
Cmpd 47	STP Peak 85	Branched Alkene	17.56	145	0.031
Cmpd 48	STP Peak 86	Branched Alkene	17.74	97	0.182
Cmpd 49	STP Peak 6	3-Isopropylphenol	17.81	121	0.300
Cmpd 50	STP Peak 54	Dichlorobenzonitrile	17.99	171	0.180
Cmpd 51	STP Peak 32	Unidentified Hydrocarbon	18.33	122	0.093
Cmpd 52	STP Peak 45	Branched Alkane	18.69	172	0.021
Cmpd 53	STP Peak 61a	Alkyl Indan	19.07	145	0.140
Cmpd 54	STP Peak 61b	Phenoxyacetic Acid	19.14	152	0.161
Cmpd 55	STP Peak 46	2,6-*t*-Butylphenol	20.06	191	0.181

Table 3. Compounds in municipal STP effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 56	STP Peak 87	Benzopyran-2-one	20.19	146	0.155
Cmpd 57	STP Peak 15	Diethyl phthalate	20.21	149	0.519
Cmpd 58	STP Peak 62	γ-Methylionone	21.01	135	0.185
Cmpd 59	STP Peak 64	Unidentified Oxy Hydrocarbon	21.42	101	0.111
Cmpd 60	STP Peak 63	2,6-Bis(1,1-dimethylethyl)-4-methylphenol	21.67	205	0.185
Cmpd 61	STP Peak 7	N,N-Diethyl-3-methyl Benzamide	23.15	119	0.350
Cmpd 62	STP Peak 65	Alkane	23.31	57	0.173
Cmpd 63	STP Peak 8	Dibutylphthalate	23.38	149	0.384
Cmpd 64	STP Peak 66	Unidentified Oxy Hydrocarbon	23.42	71	0.267
Cmpd 65	STP Peak 55	2-(Methylthio)benzothiazole	23.68	181	0.151
Cmpd 66	STP Peak 47	Tributylphosphate	24.39	99	0.364
Cmpd 67	STP Peak 67	Unidentified Amine	25.26	205	0.131
Cmpd 68	STP Peak 68	Alkane	25.41	57	0.144
Cmpd 69	STP Peak 9	Unidentified	25.83	98	0.237
Cmpd 70	STP Peak 10a	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine	26.39	201	0.059
Cmpd 71	STP Peak 10b	Nonyl Phenol Isomer	26.42	121	0.140
Cmpd 72	STP Peak 11	Nonyl Phenol Isomer	26.55	135	0.253
Cmpd 73	STP Peak 12	Nonyl Phenol Isomer	26.68	135	0.141
Cmpd 74	STP Peak 69	2-Chloroethylphosphate	26.74	249	0.034
Cmpd 75	STP Peak 71	Unidentified	27.43	125	0.118
Cmpd 76	STP Peak 70	Nonylphenol Isomer	27.52	135	0.278
Cmpd 77	STP Peak 72	Neophytadiene	27.90	123	0.044
Cmpd 78	STP Peak 73	Unidentified	28.45	243	0.116
Cmpd 79	STP Peak 13	Caffeine	28.50	194	0.183
Cmpd 80	STP Peak 14	Unidentified Diterpene	28.65	243	0.074
Cmpd 81	STP Peak 48	Hexadecanoic Acid	30.07	129	0.044
Cmpd 82	STP Peak 49	Oleic Acid	33.02	83	0.061

Table 3. Compounds in municipal STP effluents (continued).

Compound Number	Peak Number	Compound Name, Formula or Description	Adjusted Retention Time	Q Ion	Quant Factor
Cmpd 83	STP Peak 50	Stearic Acid	33.34	129	0.036
Cmpd 84	STP Peak 57	1,3-Dichloro-iso-propylphosphate	35.98	191	0.054
Cmpd 85	STP Peak 16	Butylphenyl phthalate	36.31	149	0.161
Cmpd 86	STP Peak 17	2-Butoxyethyl phosphate	37.08	125	0.073
Cmpd 87	STP Peak 74	Diheptyphosphate	38.76	149	0.472
Cmpd 88	STP Peak 18	Bis(ethylhexyl)phthalate	38.89	149	0.265
Cmpd 89	STP Peak 75	Sterol	42.26	370	0.025
Cmpd 90	STP Peak 19	Squalene	42.49	81	0.126
Cmpd 91	STP Peak 20	Unidentified Sterol	46.72	386	0.020

Table 4. Anthropogenic compounds identified in Slave Lake Pulp Company effluent (concentrations in ug/L).

Date Sampled	21-Feb-91	20-Jun-91	23-Jul-91	15-Aug-91	6-Nov-91	11-Feb-92	9-Mar-92	13-Mar-92	29-Apr-92	9-Mar-92	17-Nov-92	10-Jun-93	18-Aug-93	28-Oct-93
2,2'-Azobis[2-methylpropanenitrile]	173	24	13	13	nd	25	26	20	10	nd	7	nd	nd	nd
Benzothiazole	nd	nd	109	24	nd	nd	nd	nd	13	nd	nd	nd	nd	nd
Benzeneacetic Acid	565	357	52	72	992	nd	91	765	nd	nd	nd	nd	nd	nd
Indole	315	76	nd	31	407	nd	302	1322	nd	nd	nd	nd	nd	nd
Alkyl Phenol	nd	32	15	57	nd	nd	2983	2079	nd	nd	nd	nd	nd	nd
2-(Methylthio)benzothiazole	nd	nd	62	25	nd	nd	18	nd	nd	nd	nd	nd	nd	nd
Diphenylamine	nd	nd	46	42	nd	nd	19	22	nd	nd	nd	nd	nd	nd
N-Butyl-benzenesulphonamide	nd	nd	961	257	nd	nd	398	130	360	nd	nd	nd	nd	nd
N-Phenylbenzamide	nd	nd	100	53	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd

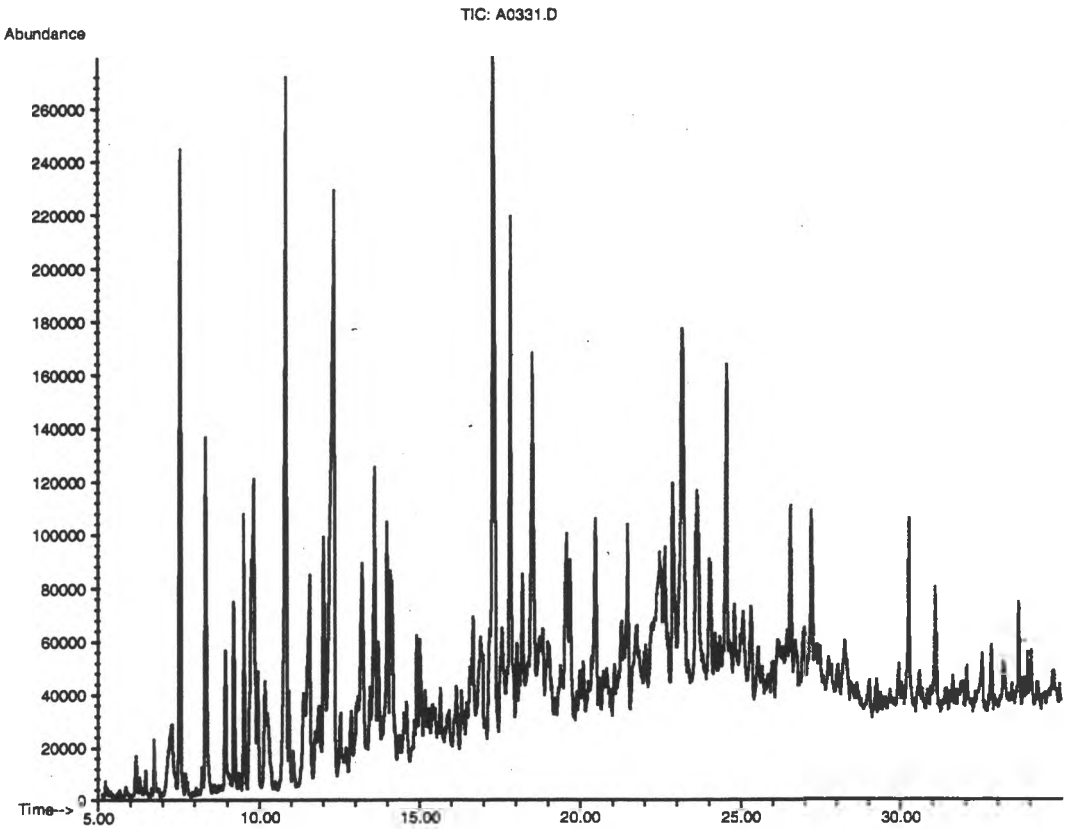


Figure 1. TIC of kraft mill effluent sampled in 1991, typical of conventional BKME.

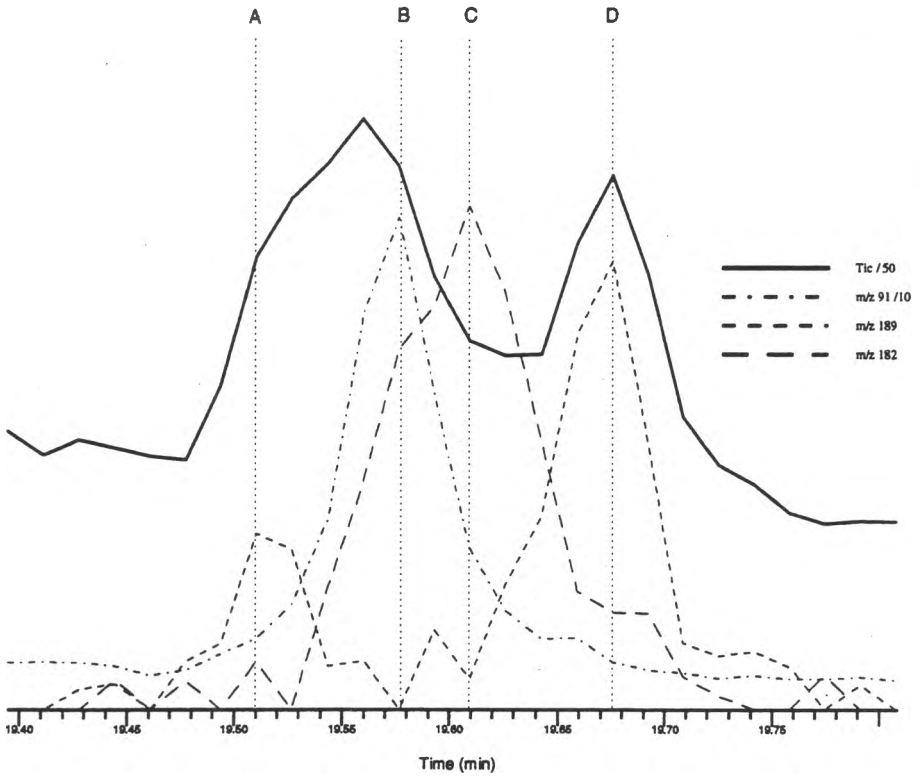


Figure 2. Small region of above BKME TIC with extracted ion chromatograms of ions representative of underlying compounds.

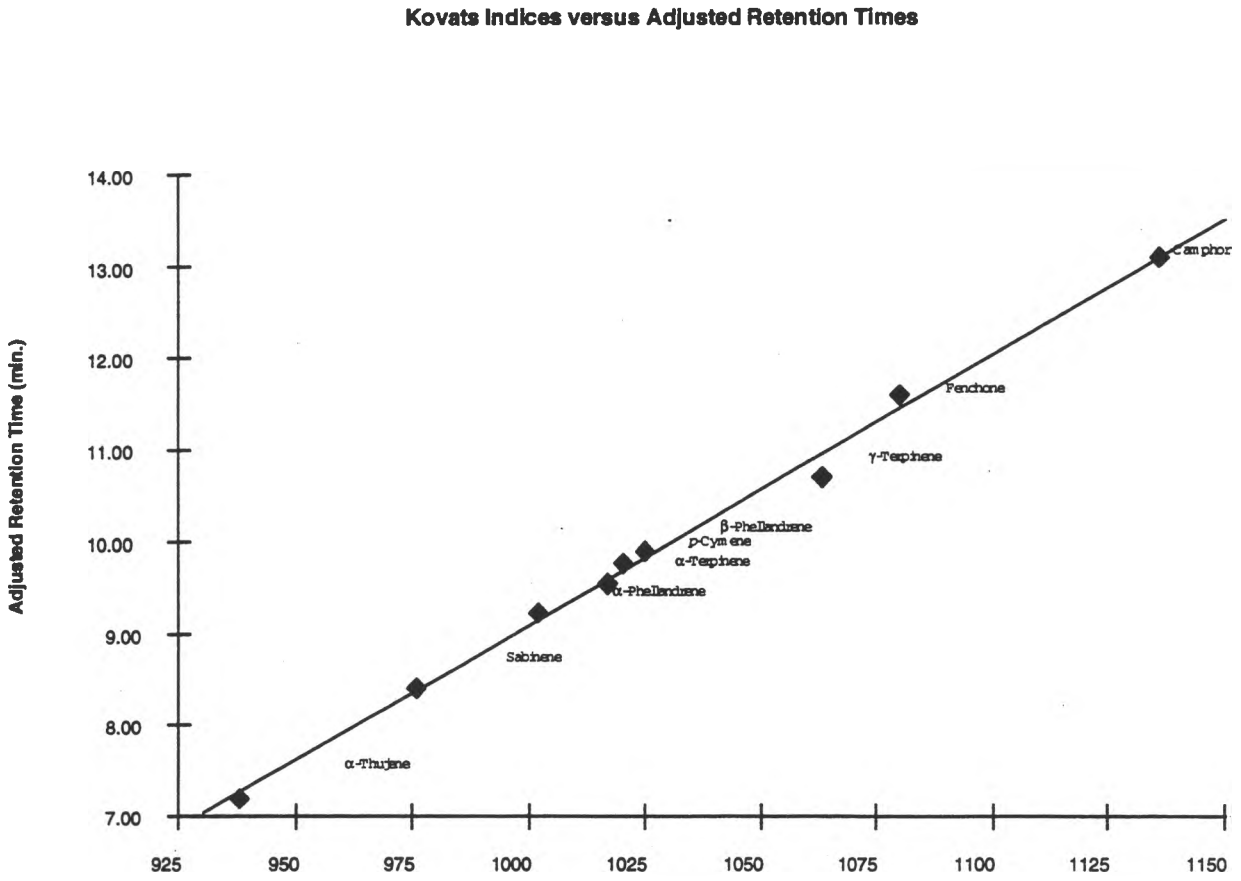


Figure 3. Plot of Kovats Indices versus adjusted retention times for monoterpenes identified in BKME and CTMP effluents.

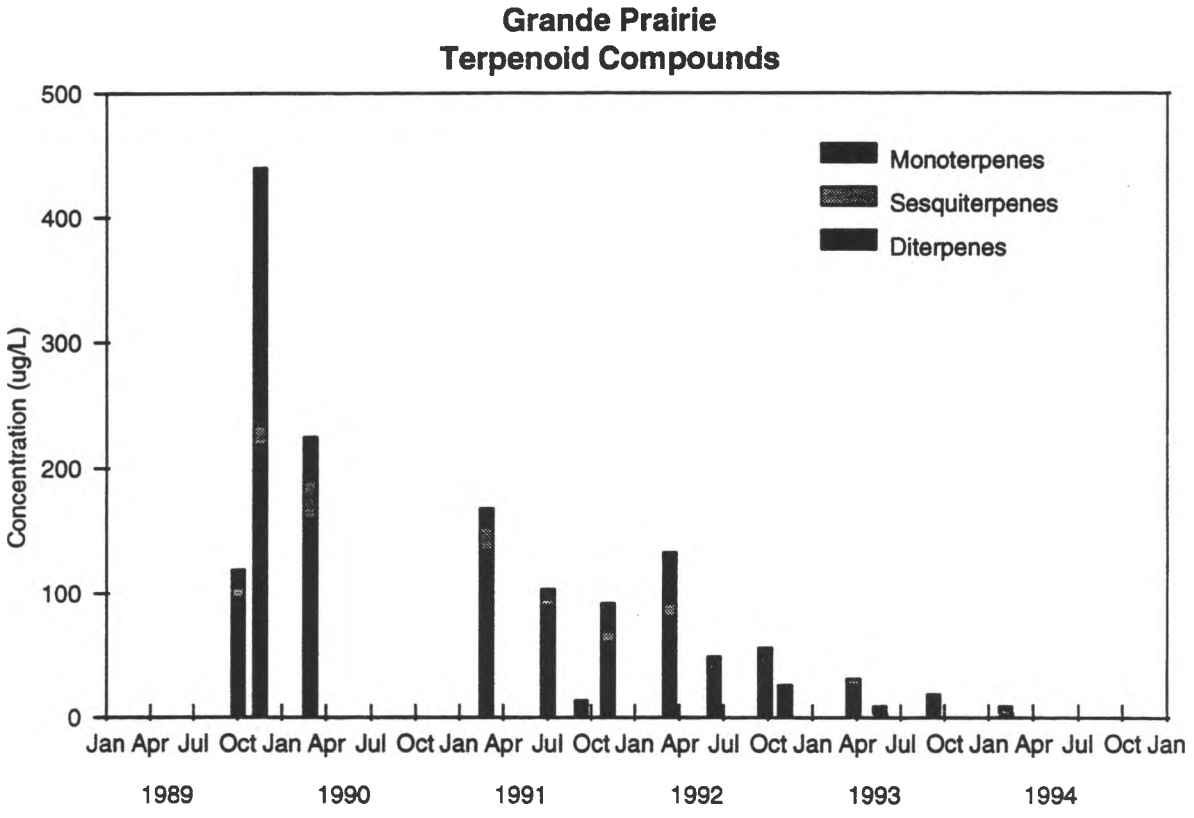


Figure 4. Terpenoid compounds in the Grande Prairie mill effluent.

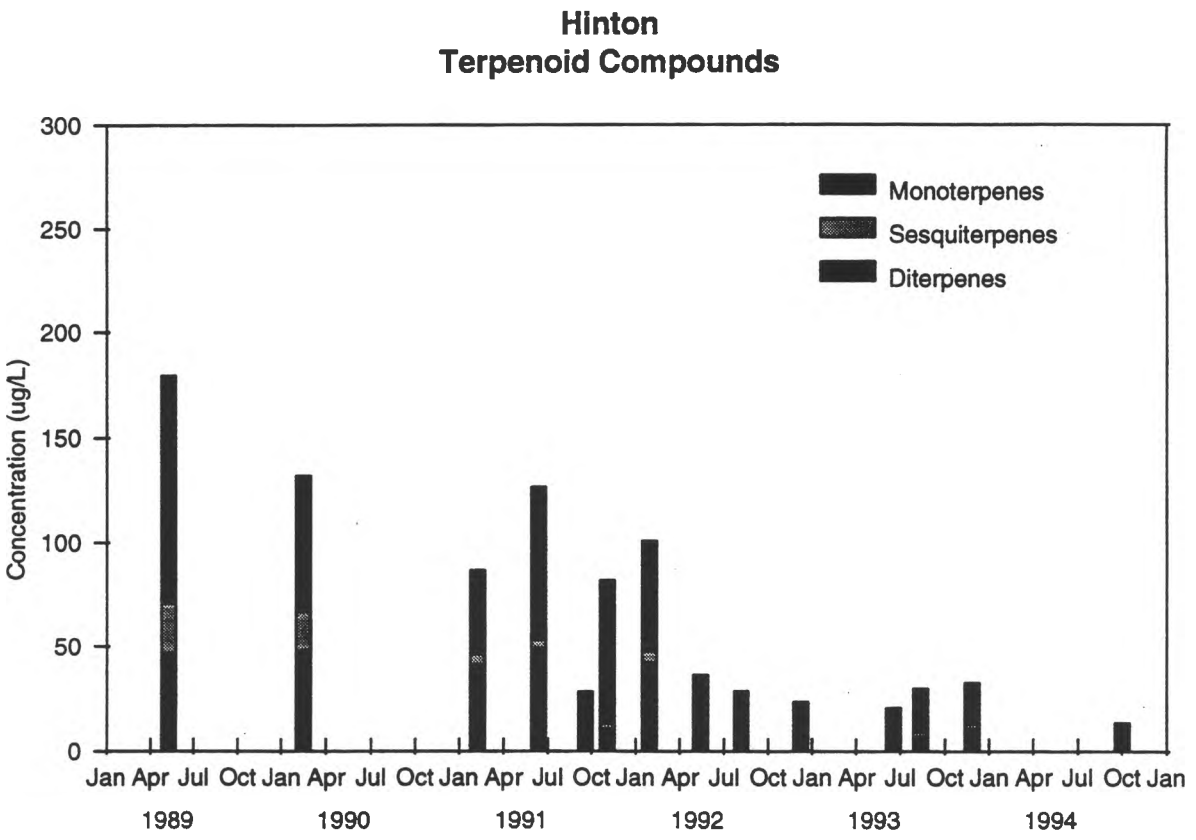


Figure 5. Terpenoid compounds in the Hinton mill effluent.

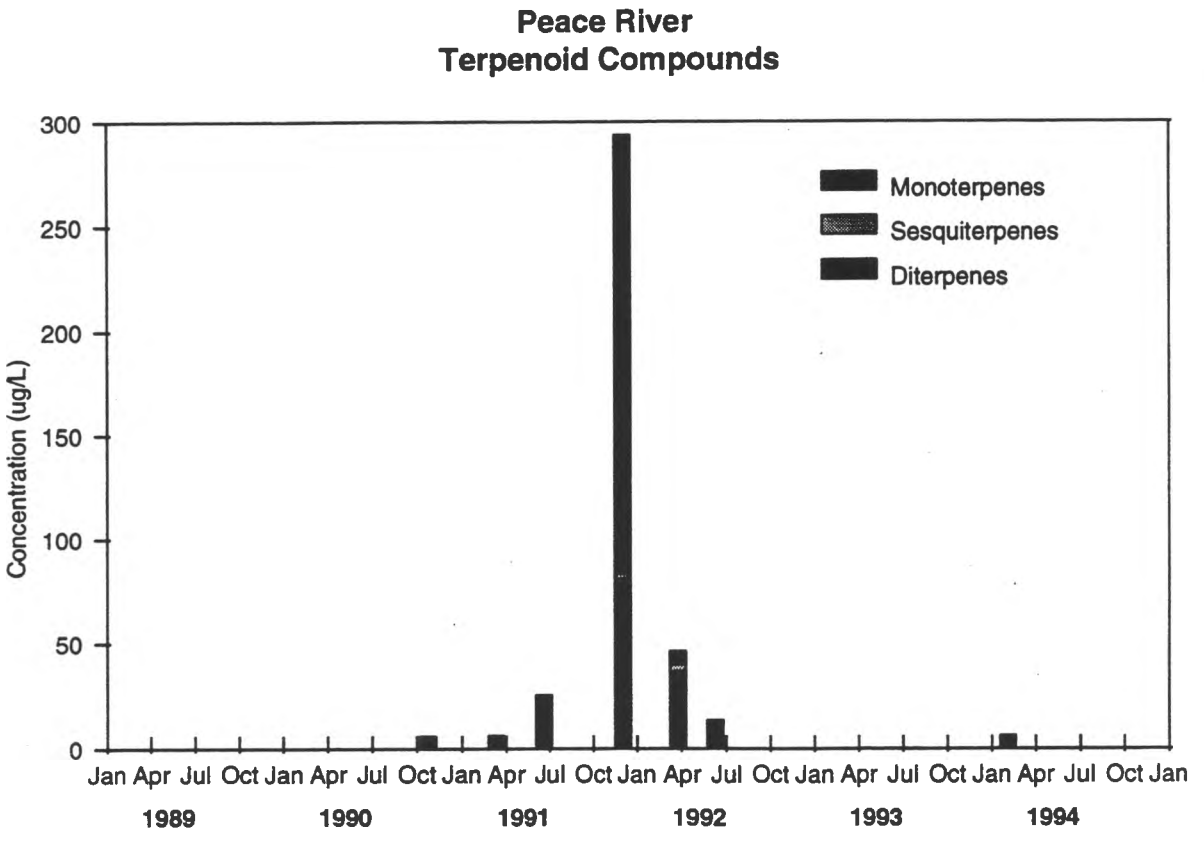


Figure 6. Terpenoid compounds in the Peace River mill effluent.

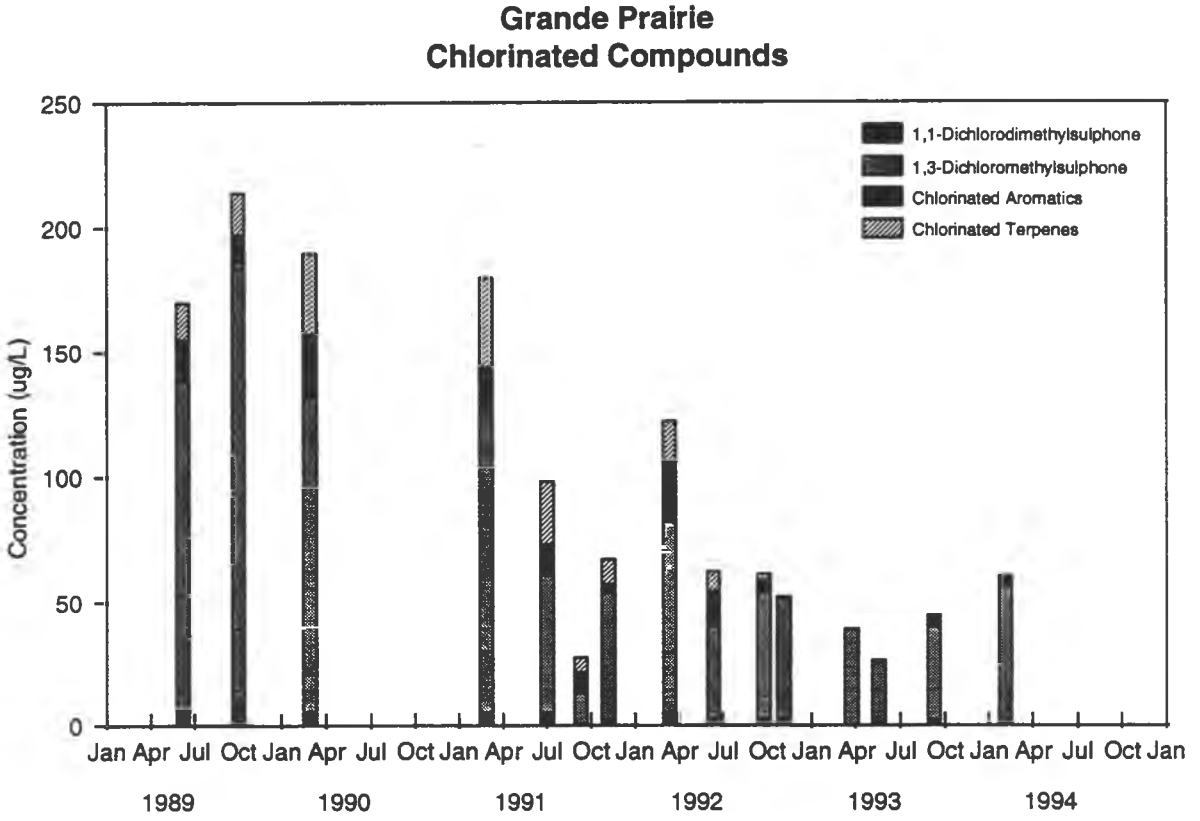


Figure 7. Chlorinated compounds in the Grande Prairie mill effluent.

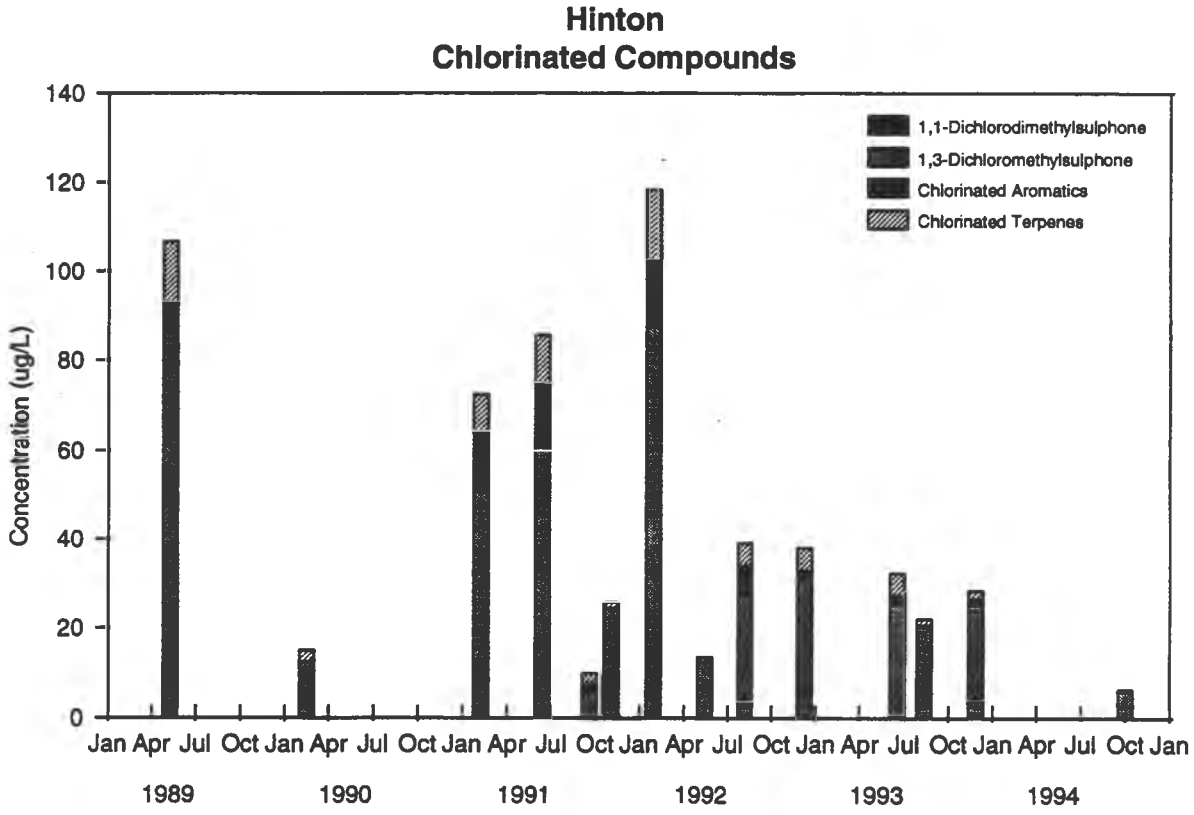


Figure 8. Chlorinated compounds in the Hinton mill effluent.

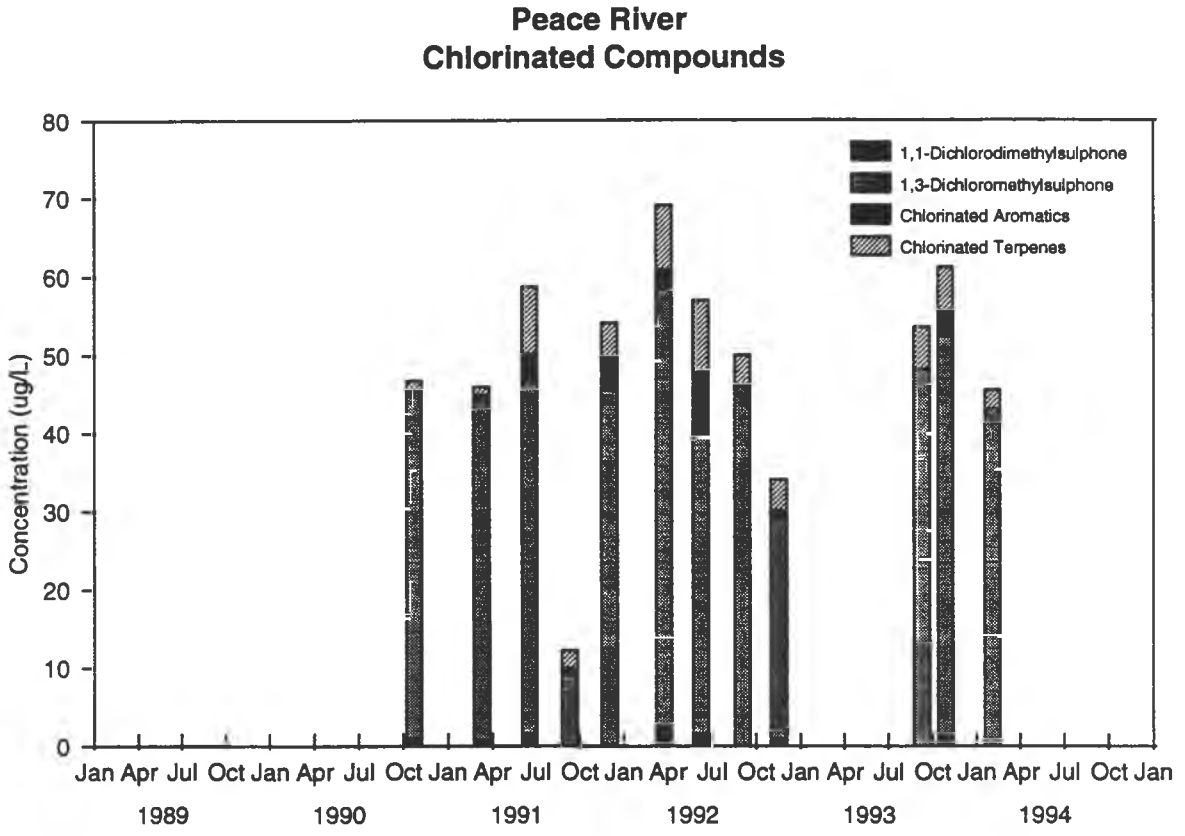


Figure 9. Chlorinated compounds in the Peace River mill effluent.

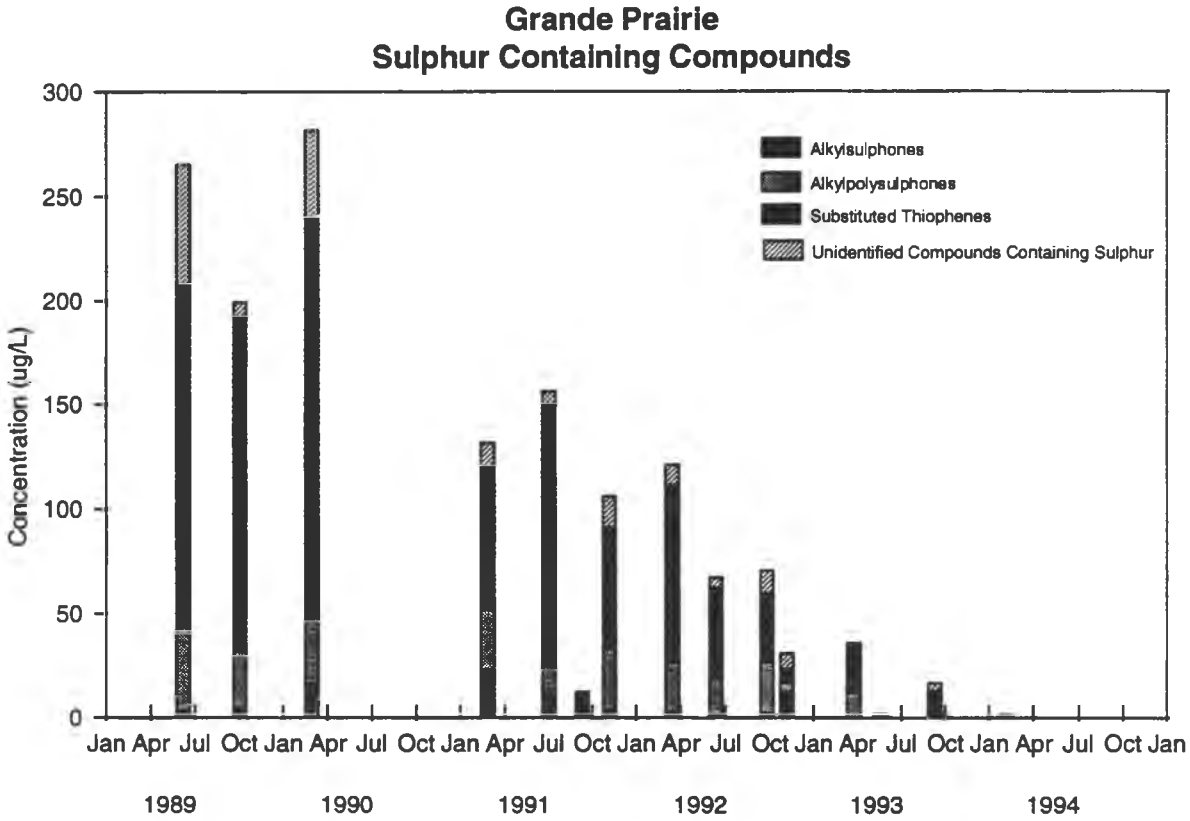


Figure 10. Sulphur containing compounds in the Grande Prairie mill effluent.

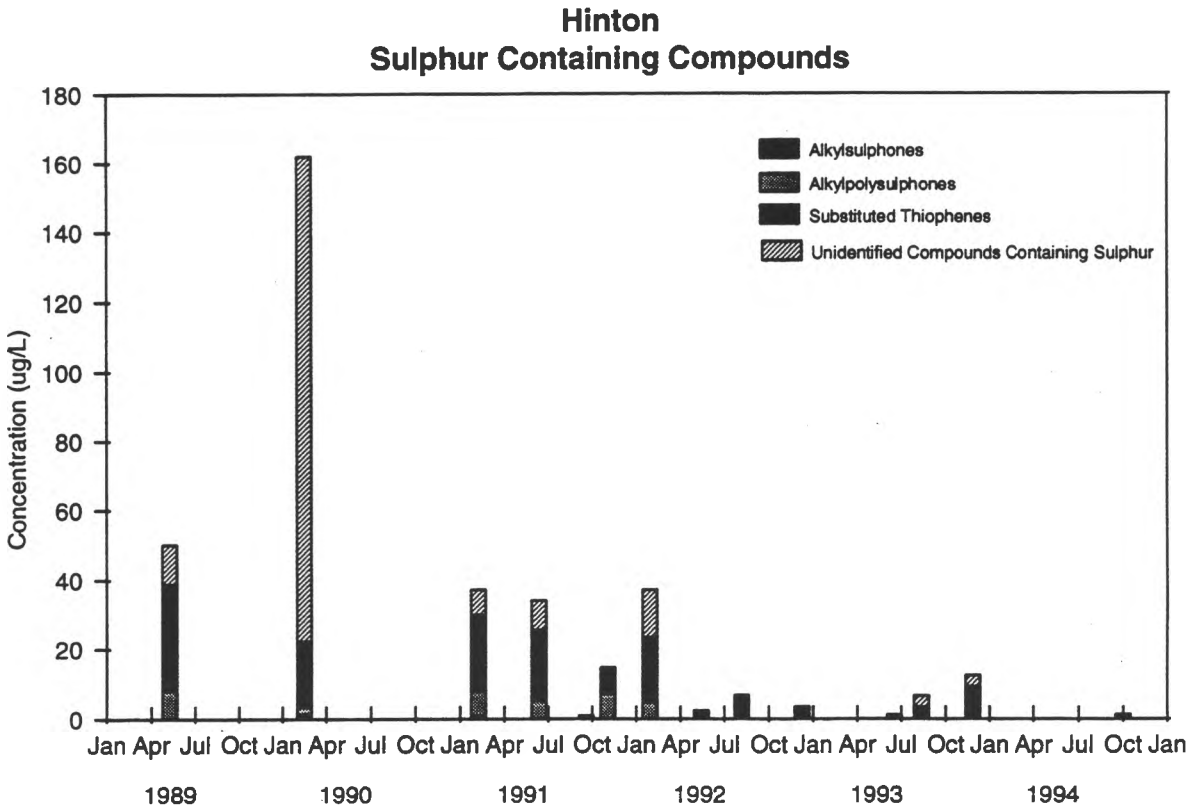


Figure 11. Sulphur containing compounds in the Hinton mill effluent.

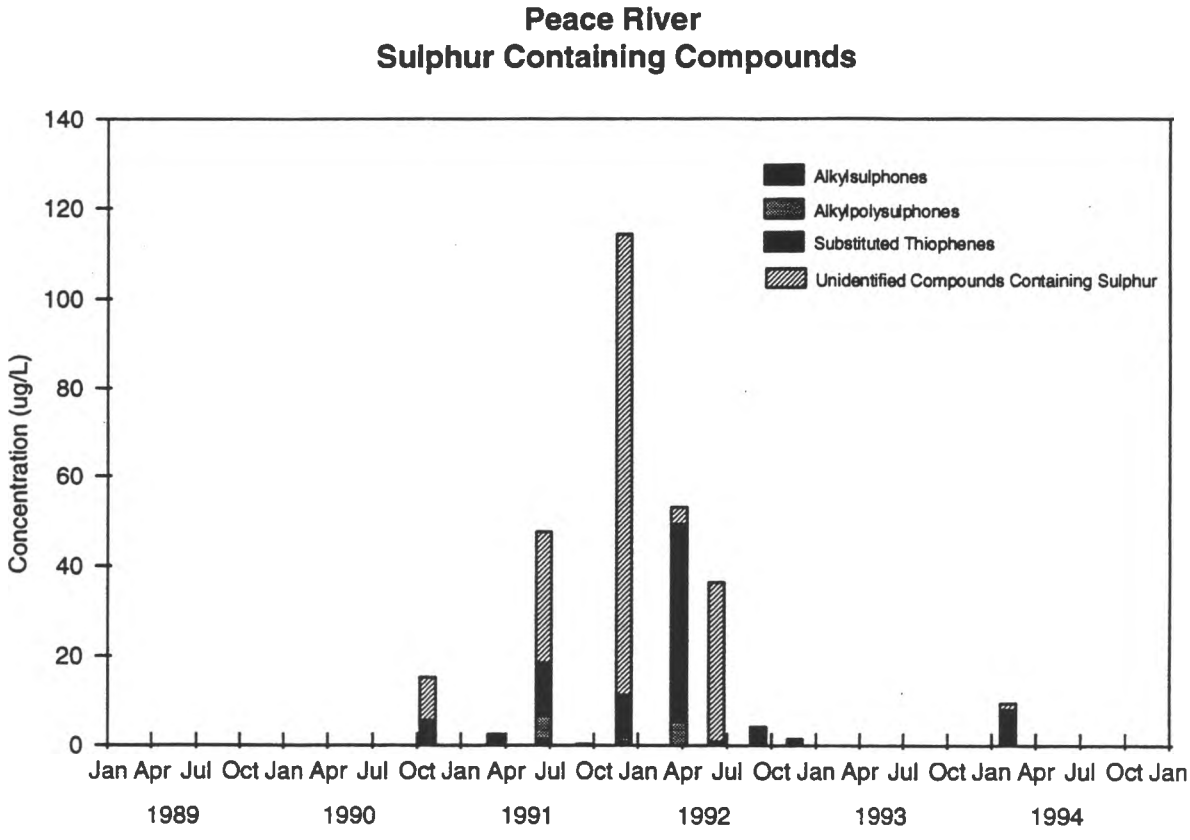


Figure 12. Sulphur containing compounds in the Peace River mill effluent.

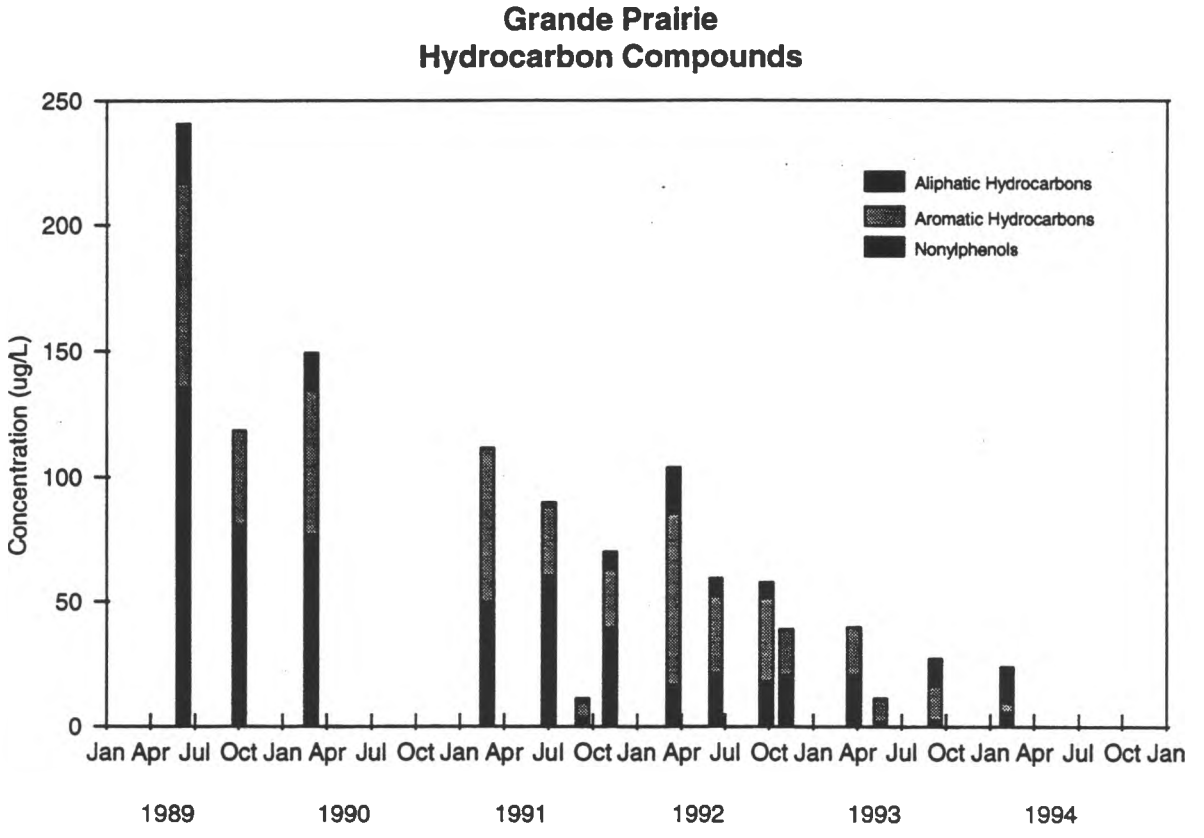


Figure 13. Hydrocarbon compounds in the Grande Prairie mill effluent.

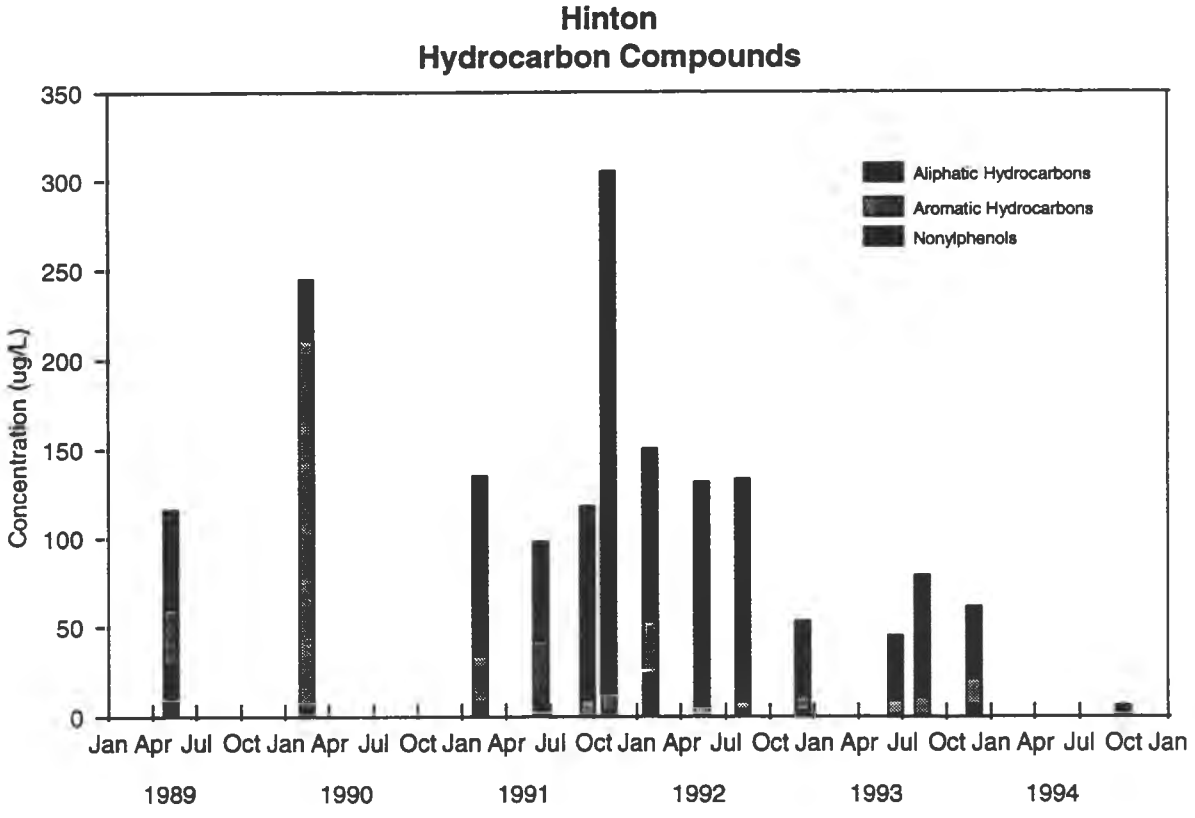


Figure 14. Hydrocarbon compounds in the Hinton mill effluent.

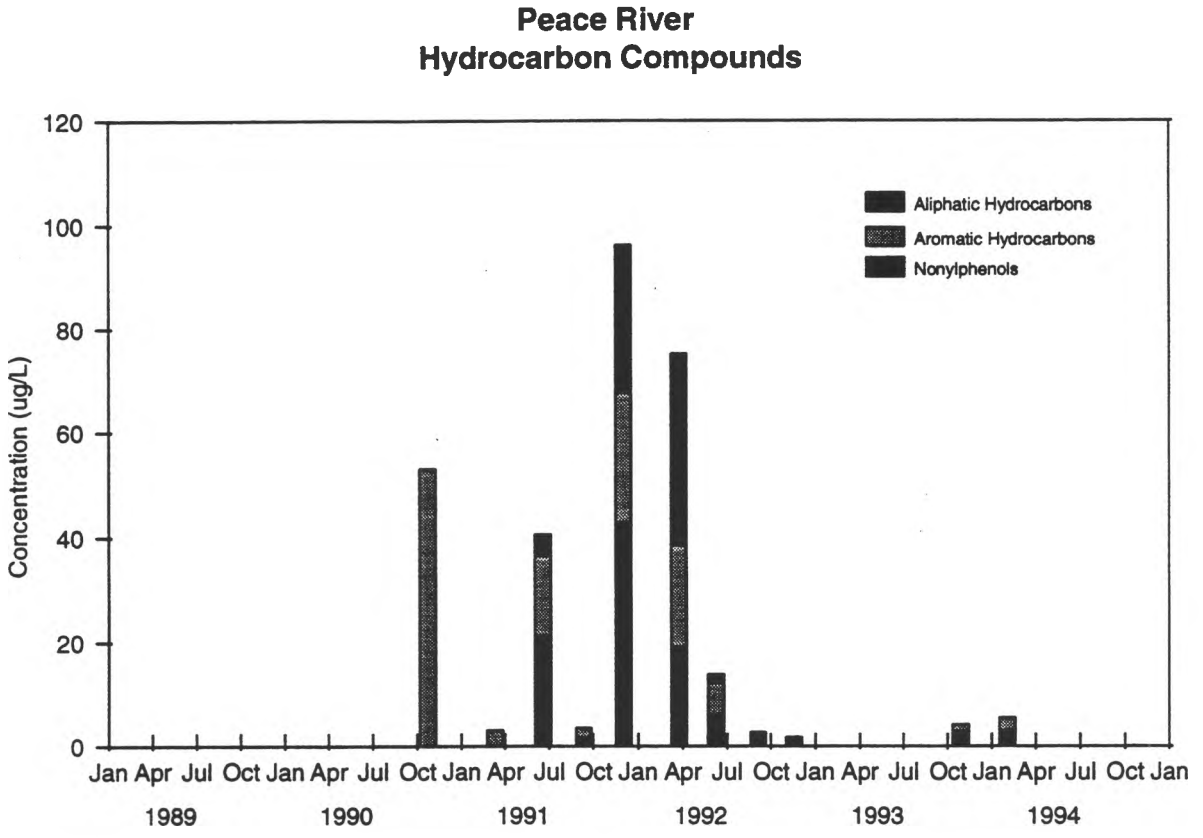


Figure 15. Hydrocarbon compounds in the Peace River mill effluent.

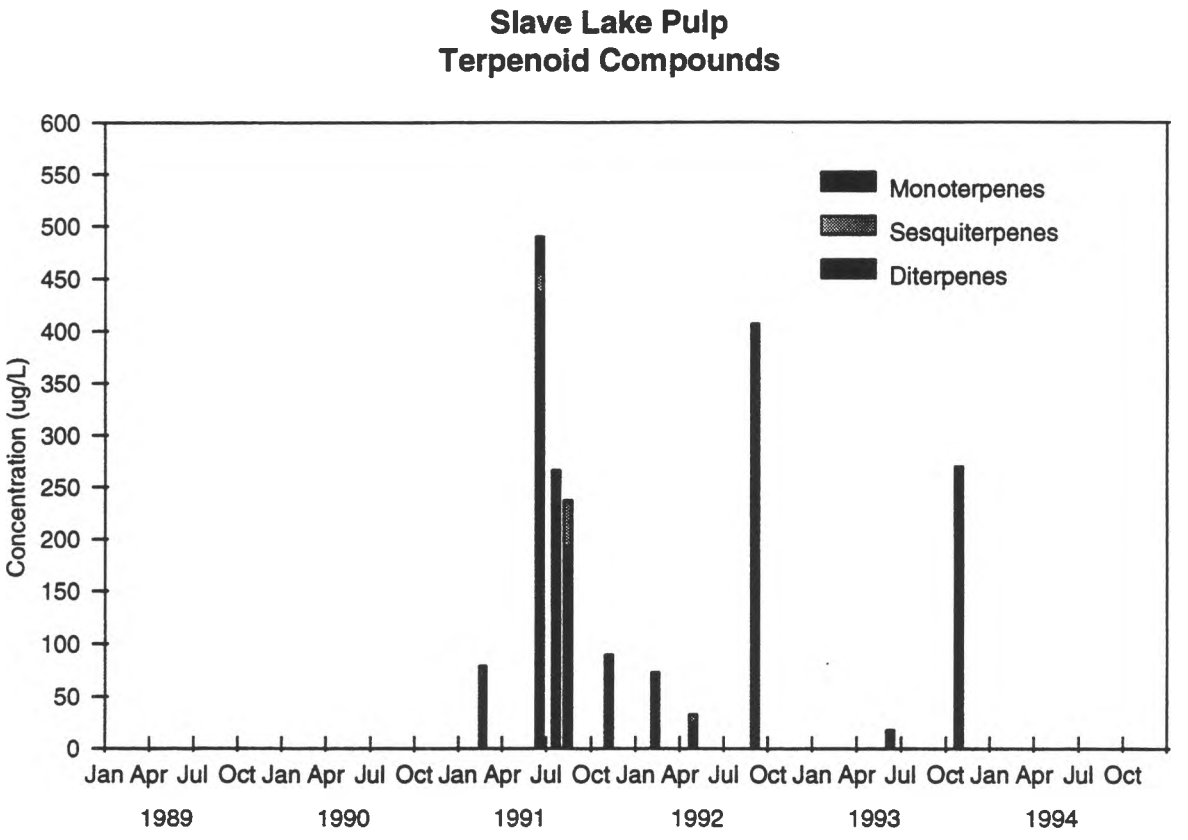


Figure 16. Terpenoid compounds in the Slave Lake mill effluent.

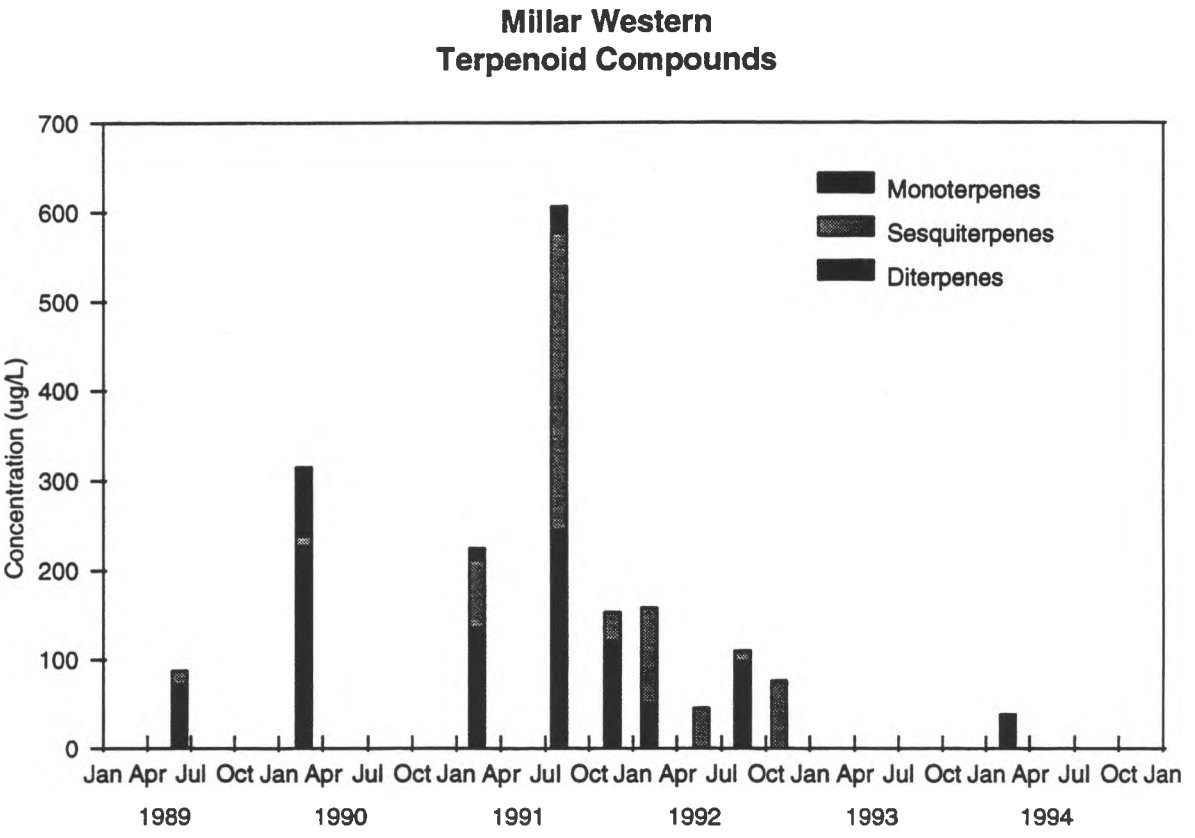


Figure 17. Terpenoid compounds in the Millar Western mill effluent.

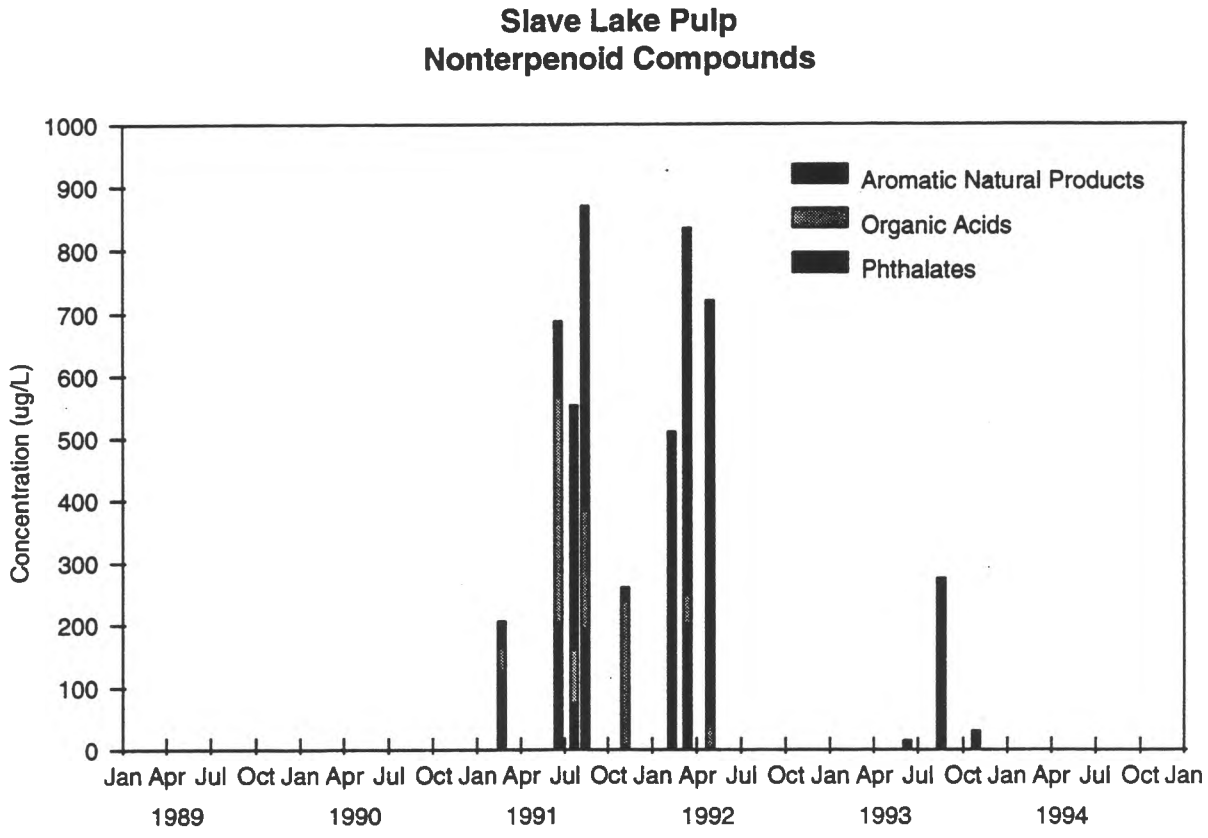


Figure 18. Nonterpenoid compounds in the Slave Lake mill effluent.

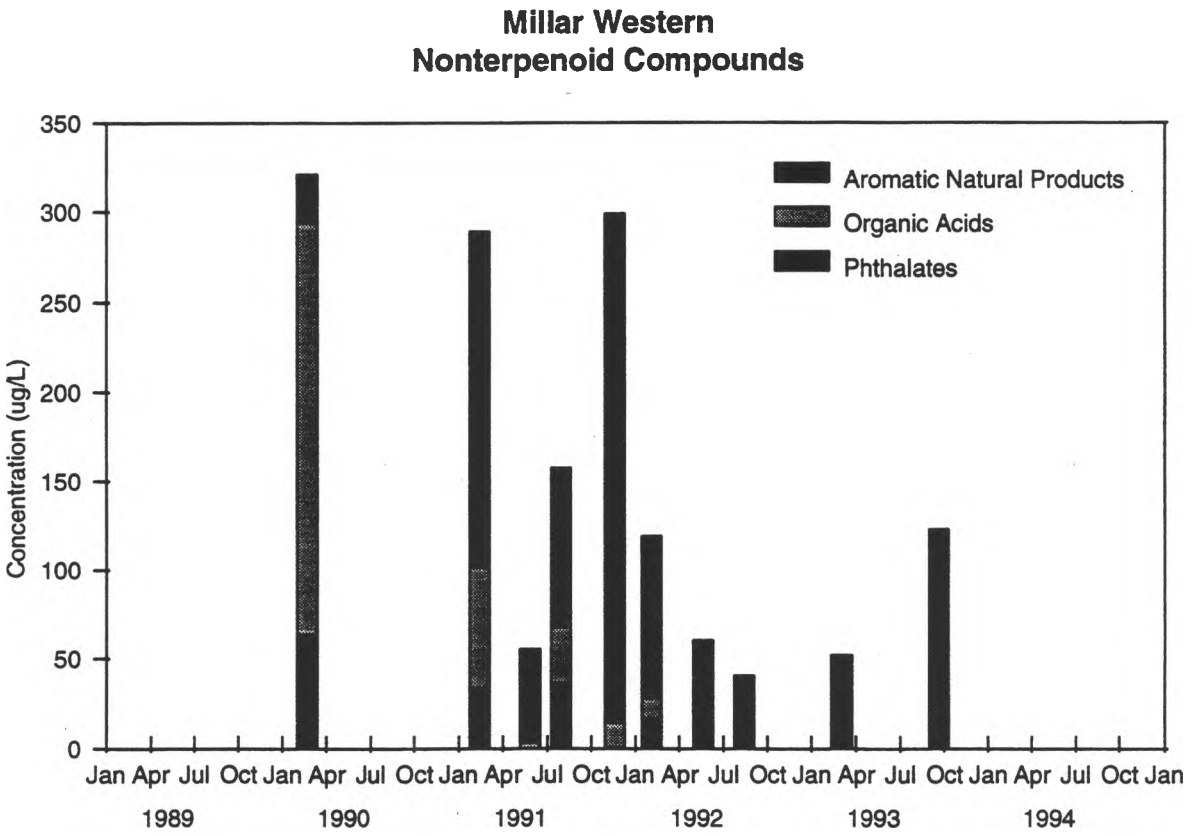


Figure 19. Nonterpenoid compounds in the Millar Western mill effluent.

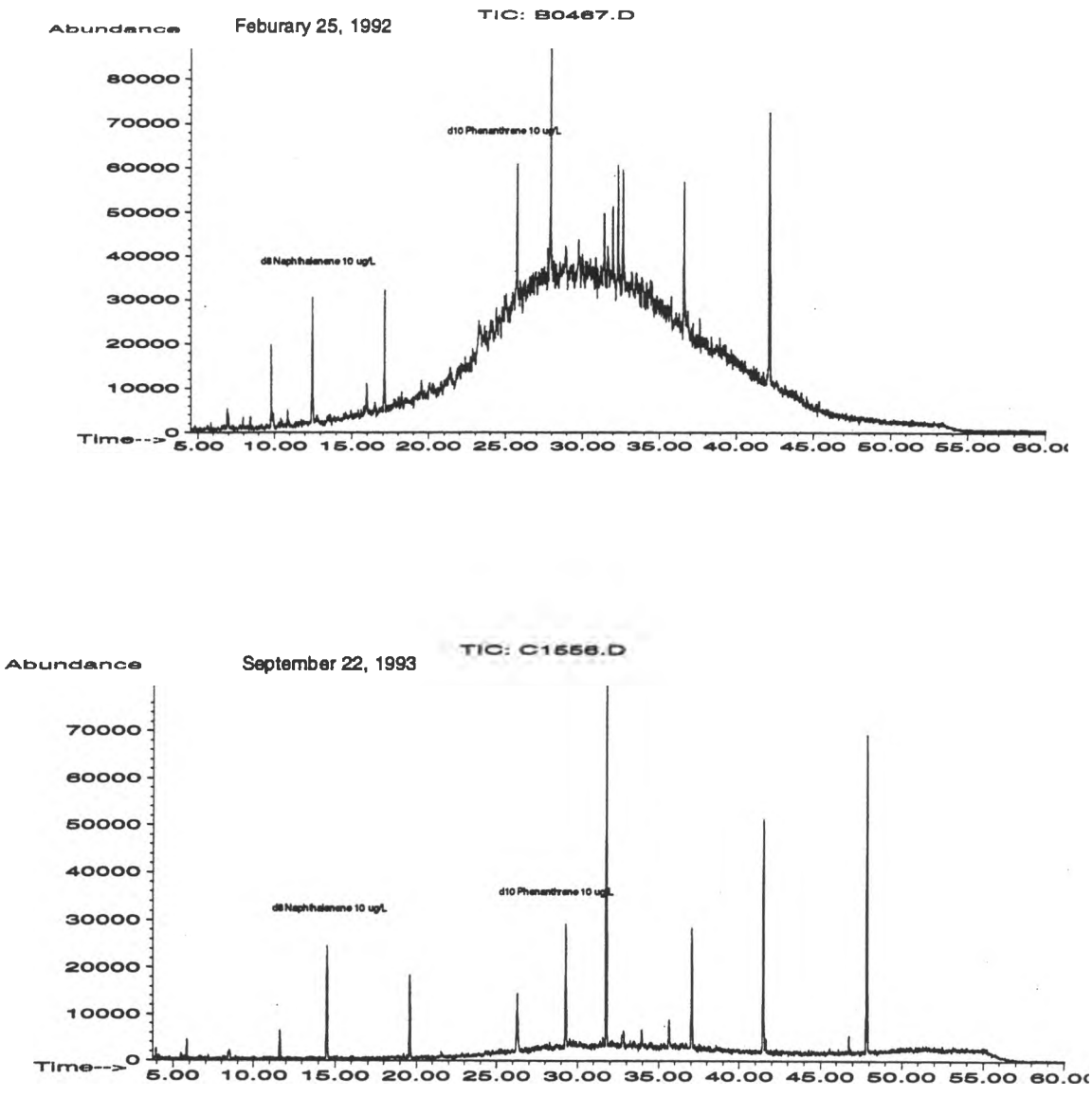


Figure 20. Total ion chromatograms of extracts of the Suncor process effluent taken in 1992 and 1993.

APPENDIX A: BROAD SPECTRUM ANALYSIS OF MUNICIPAL AND INDUSTRIAL EFFLUENT DISCHARGED INTO THE PEACE, ATHABASCA AND SLAVE RIVER BASINS - DATABASE FILES

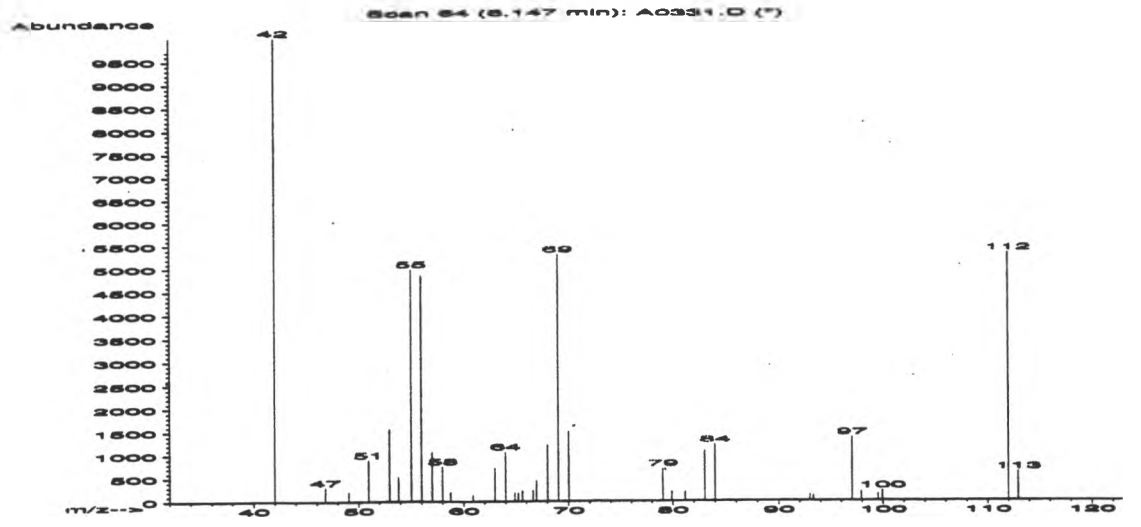
This report was split into three separate project reports; namely, Northern River Basins Study (NRBS) Project Report No's 138, 121 and 111. An electronic copy of these three reports and their appendices (where electronic copies exist) are contained on the three disks provided in NRBS Project Report No. 138. This information is being provided to facilitate use by researchers. Users are encouraged to contact the authors of these reports for additional background information.

There is no warranty expressed or implied for the use of this database; the Northern River Basins Study does not guarantee the accuracy of the data. The NRBS does not assume any liability for actions or consequences resulting from the use of the data; individuals using this data do so entirely at their own risk. The NRBS will not update the data except as deemed necessary for its own purpose.

APPENDIX 1

MASS SPECTRAL DATA OF COMPOUNDS IN BLEACHED KRAFT MILL EFFLUENTS

Peak 1



Scan 64 (6.147 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	10000	60.90	129	79.05	691	112.00	5328
46.80	297	63.00	711	79.90	193	112.90	619
49.05	204	64.00	1064	81.15	190		
50.95	887	64.90	179	83.00	1078		
52.95	1562	65.25	176	84.00	1218		
53.80	521	65.65	221	92.95	132		
55.05	4983	66.65	232	93.30	104		
56.00	4835	67.00	445	97.05	1369		
57.00	1064	68.05	1212	97.95	185		
58.00	747	69.05	5300	99.55	140		
58.75	193	70.05	1503	99.95	216		

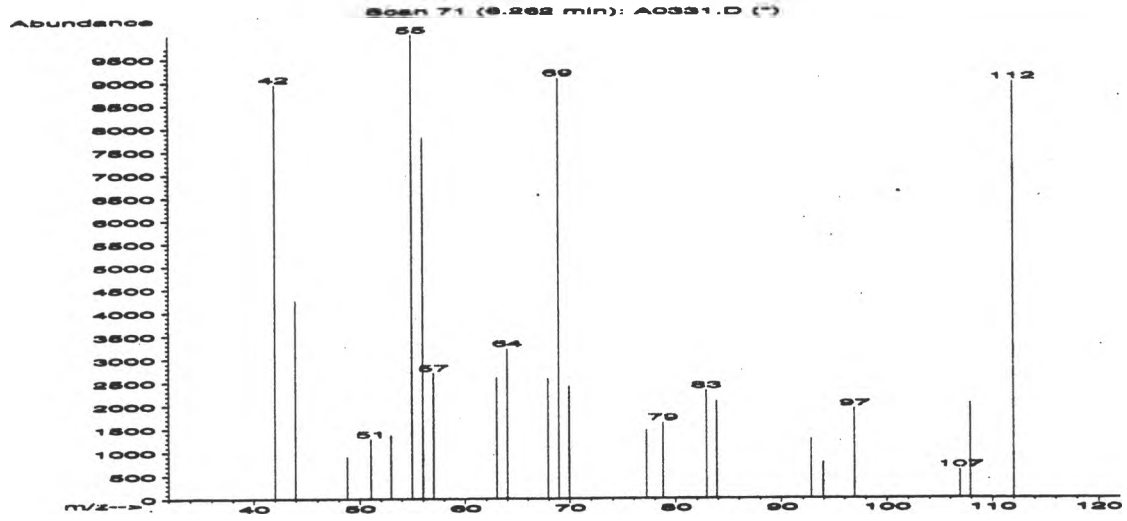
Scan 64 (6.147 min): A0331.D

Compounds from Proctor and Gamble A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	83
2.	1,4-Diazabicyclo[2.2.2]octane	112	C6H12N2	80
3.	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	74
4.	1-Pyrrolidinamine, N-ethylidene-	112	C6H12N2	53
5.	1,3-Cyclohexanedione	112	C6H8O2	50
6.	1,4-Diazabicyclo[2.2.2]octane	112	C6H12N2	50
7.	Cyclooctane	112	C8H16	47
8.	1,4-Diazabicyclo[2.2.2]octane	112	C6H12N2	47
9.	3-HEPTENE, 2-METHYL-	112	C8H16	46
10.	QUINUCLIDINE-4-D	111	C7H12DN	40
11.	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	40
12.	Heptane, 4-methylene-	112	C8H16	35
13.	1,3-Cyclopentanedione, 2-methyl-	112	C6H8O2	32
14.	4-Pentenal, 2-methyl-	98	C6H10O	27
15.	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	112	C6H8O2	25
16.	QUINUCLIDINE-3-D	111	C7H12DN	22
17.	N'-Cyano-N,N-dimethyl-guanidine	112	C4H8N4	22
18.	Phenol, 3-fluoro-	112	C6H5FO	18
19.	2-Hexene, 2,5-dimethyl-	112	C8H16	18
20.	1-Nonanol	144	C9H20O	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	013368-65-5	119033	60	17	0	74	14	50	26	55	8348
2.	*80	000280-57-9	2530	51	53	2	95	12	48	0	46	9103
3.	*74	013368-65-5	119032	58	45	1	79	16	44	10	50	7885
4.	*53	060144-27-6	2526	39	59	0	77	30	28	0	39	8813
5.	*50	000504-02-9	2488	33	50	1	99	32	25	0	39	8574
6.	*50	000280-57-9	119013	45	64	2	53	35	25	0	40	8813
7.	*47	000292-64-8	2729	33	76	3	168	40	20	0	39	8046
8.	*47	000280-57-9	119012	44	64	1	51	36	20	0	39	8977
9.	*46	000000-00-0	119062	59	35	1	47	45	20	20	49	6481
10.	40	033513-69-8	2378	44	55	1	88	35	16	0	37	9025
11.	*40	013368-65-5	2569	51	59	1	105	33	16	2	35	8441
12.	*35	015918-08-8	2684	37	68	3	222	53	11	0	41	5859
13.	*32	000765-69-5	2473	39	52	2	48	50	9	6	35	5711
14.	*27	005187-71-3	781	39	52	2	168	56	8	0	39	8590
15.	*25	000080-71-7	2469	36	60	2	43	54	7	2	35	6282
16.	*22	033259-52-8	2379	35	63	3	177	62	5	0	39	8693
17.	*22	000000-00-0	2412	39	30	0	53	62	5	0	39	6459
18.	*18	000372-20-3	2445	37	42	0	37	66	3	18	43	4138
19.	*18	003404-78-2	119074	37	48	0	52	66	3	10	43	5758
20.	16	000143-08-8	122961	43	71	2	52	57	3	0	37	7309



Scan 71 (6.262 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	8955	68.95	9058	112.00	8968		
43.95	4258	69.95	2413				
48.80	903	77.20	1458				
51.05	1277	78.80	1626				
52.95	1355	82.90	2323				
54.95	10000	83.90	2090				
56.00	7755	92.80	1265				
57.00	2697	93.95	774				
63.00	2594	96.95	1923				
64.00	3213	106.90	606				
67.95	2581	107.90	2026				

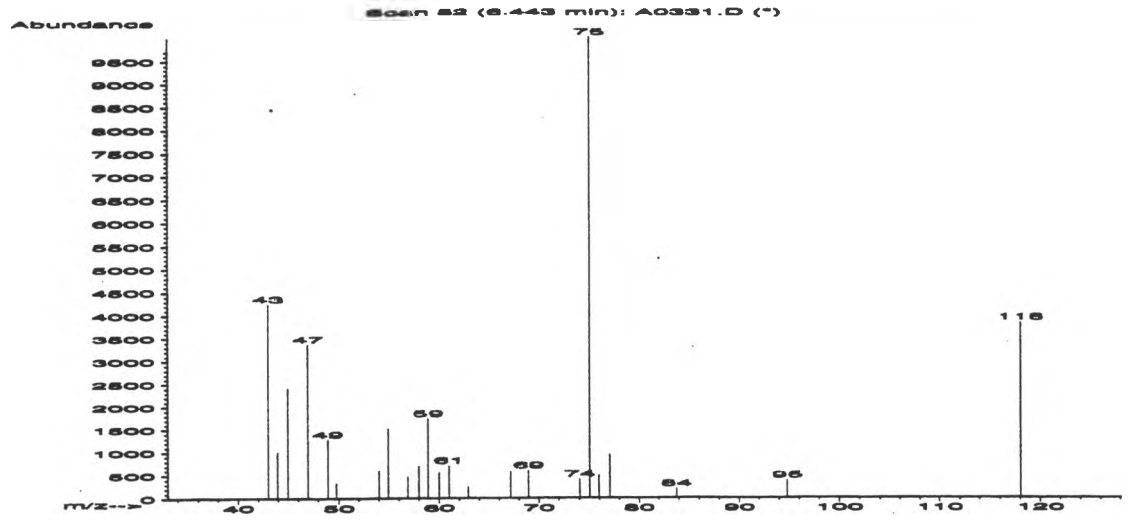
Scan 71 (6.262 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	43
2.	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	43
3.	2,5-DIMETHYL-.DELTA.'-PYRROLINE	97	C6H11N	38
4.	3-Octene, (Z)-	112	C8H16	37
5.	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	35
6.	Cyclohexane, 1,4-dimethyl-, cis-	112	C8H16	35
7.	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	35
8.	2-HEXENE, 3,5-DIMETHYL-	112	C8H16	35
9.	Isooctanol	130	C8H18O	32
10.	Cyclohexanone, 4-methyl-	112	C7H12O	27
11.	Cyclooctane	112	C8H16	25
12.	1-Heptene, 2-methyl-	112	C8H16	25
13.	3-Hexene, 2,5-dimethyl-, (E)-	112	C8H16	22
14.	Cyclohexanone, 3-methyl-, (R)-	112	C7H12O	22
15.	Cyclooctane	112	C8H16	17
16.	Cyclopropane, 1-butyl-2-pentyl-, trans-	168	C12H24	17
17.	3-HEXENE, 2,5-DIMETHYL-	112	C8H16	12
18.	Pyrrolidine, 1-nitroso-	100	C4H8N2O	12
19.	1-Pentene, 3-methyl-	84	C6H12	10
20.	Cyclopentane, 1,1,2-trimethyl-	112	C8H16	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	002207-04-7	2727	34	68	2	291	43	18	11	40	5099
2.	*43	002207-01-4	2722	37	73	3	196	42	18	0	39	6206
3.	*38	000000-00-0	694	33	57	0	85	51	14	22	43	7947
4.	*37	014850-22-7	2642	40	68	2	99	42	13	7	36	8784
5.	*35	000624-29-3	119114	35	71	2	200	54	11	0	39	5236
6.	*35	000624-29-3	2726	35	71	2	200	54	11	0	39	5221
7.	*35	002207-04-7	119115	35	70	2	215	54	11	0	39	5134
8.	*35	000000-00-0	2673	35	72	3	247	51	11	0	39	8509
9.	32	026952-21-6	121210	34	31	2	99	46	9	15	33	7938
10.	*27	000589-92-4	119037	36	67	1	99	57	8	7	40	8493
11.	*25	000292-64-8	119120	39	81	2	109	51	7	14	34	8500
12.	*25	015870-10-7	119061	28	52	3	555	54	7	0	33	5667
13.	*22	000692-70-6	2681	36	63	2	174	62	5	19	40	6999
14.	*22	013368-65-5	119032	43	58	3	241	62	5	0	40	8371
15.	17	000292-64-8	2729	37	72	2	111	54	3	0	22	7550
16.	17	074663-87-9	20753	41	67	1	90	53	3	0	29	7658
17.	*12	000692-70-6	2682	40	60	2	167	62	2	8	36	7003
18.	12	000930-55-2	117893	33	89	0	71	60	2	0	25	7115
19.	*10	000760-20-3	116898	28	67	0	99	68	1	0	33	7582
20.	10	004259-00-1	2710	40	68	0	65	66	1	0	33	7500

Peak 2



Scan 82 (6.443 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4243	60.00	549	118.05	3832		
43.95	1001	61.00	706				
44.95	2413	62.90	244				
46.95	3363	67.15	574				
48.95	1277	68.95	603				
49.80	331	74.05	411				
54.05	591	75.05	10000				
54.95	1508	75.95	488				
56.90	469	77.05	937				
58.00	696	83.75	199				
58.90	1743	94.80	385				

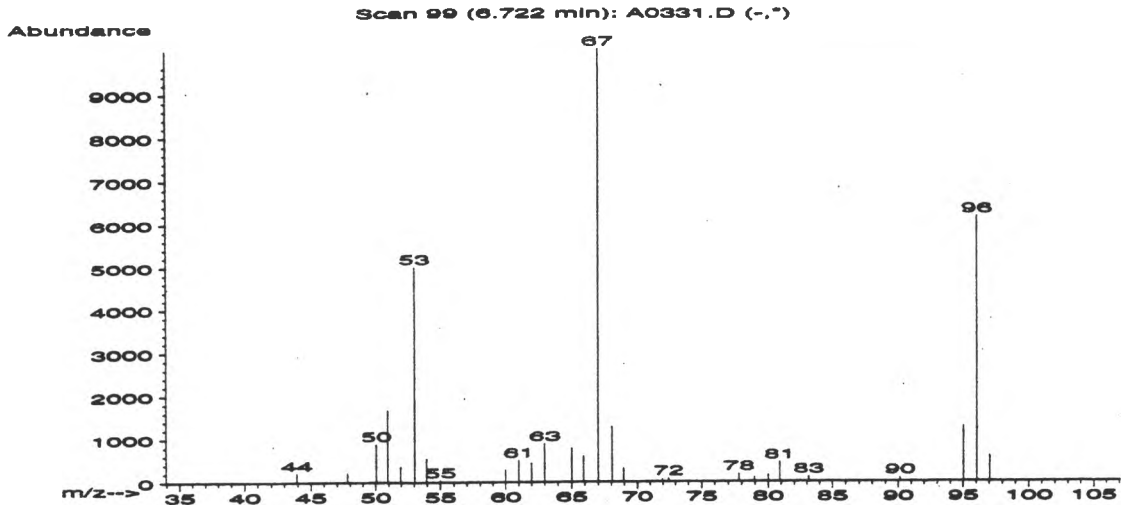
Scan 82 (6.443 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethane, 1,1-bis(methylthio)-	122	C4H10S2	53
2.	Ethane, 1,1-bis(methylthio)-	122	C4H10S2	50
3.	Butane, 2-(methylthio)-	104	C5H12S	42
4.	Ethane, 1,1-bis(methylthio)-	122	C4H10S2	40
5.	Ethanethioamide	75	C2H5NS	37
6.	2-[3'-(2'',2''-Dimethyl-6''-methylidenec	398	C22H42S2Si	17

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	53	007379-30-8	120140	44	54	0	78	29	28	2	41	9384
2.	50	007379-30-8	4298	45	63	0	85	34	25	0	39	9368
3.	42	010359-64-5	1648	47	72	1	89	29	17	0	37	9356
4.	40	007379-30-8	120141	38	56	1	70	35	16	13	31	9331
5.	*37	000062-55-5	116613	35	57	1	99	43	13	0	35	8821
6.	17	095472-42-7	97472	34	122	2	68	51	3	0	21	8601

Peak 3



Scan 99 (6.722 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	211	63.00	887	80.90	452		
47.80	216	65.00	794	83.15	119		
50.05	892	65.90	606	90.15	91		
50.95	1671	67.00	10000	95.05	1268		
51.95	353	68.05	1283	96.05	6130		
53.05	4995	68.95	314	97.05	592		
53.95	555	71.95	65				
55.00	49	72.45	76				
60.00	278	77.80	184				
61.00	509	78.95	112				
62.00	437	80.00	151				

Compounds from Proctor and Gamble A0331.D

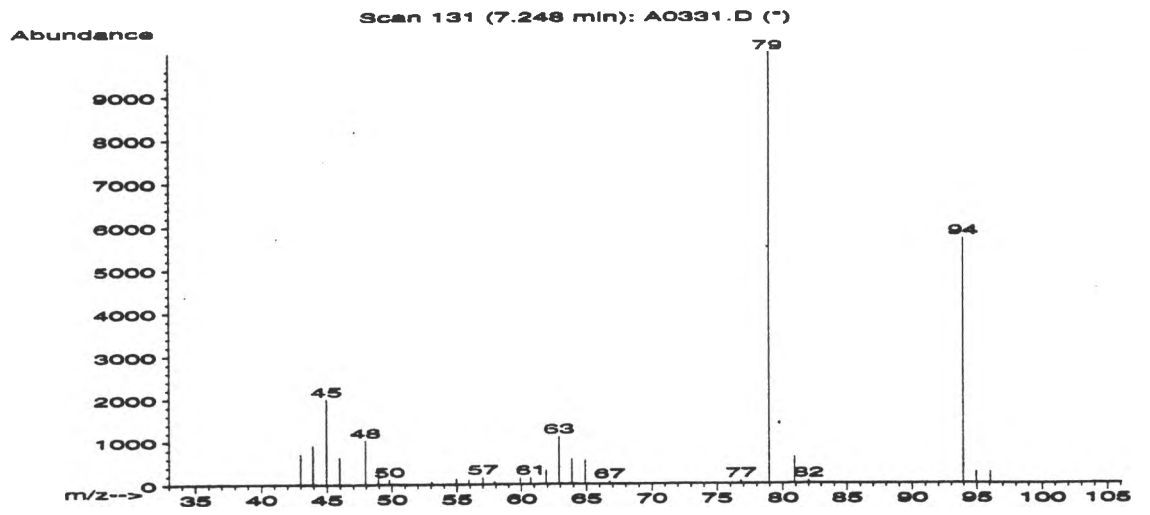
Scan 99 (6.722 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-Butenal, 2-ethenyl-	96	C6H8O	86
2.	2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	78
3.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	64
4.	2,4-DIMETHYLFURAN	96	C6H8O	64
5.	1-Pentyne	68	C5H8	59
6.	1-Pentyn-3-one, 4-methyl-	96	C6H8O	56
7.	Furan, 2,5-dimethyl-	96	C6H8O	50
8.	1,3-Pentadiene, (Z)-	68	C5H8	45
9.	1,3-Butadiene, 2-methyl-	68	C5H8	45
10.	2-Hexyne, 5-methyl-	96	C7H12	42
11.	Furan, 2,5-dimethyl-	96	C6H8O	40
12.	2,4-Hexadienal	96	C6H8O	39
13.	2,3-Hexadiene, 2-methyl-	96	C7H12	39
14.	1,4-Butanediol, 2,3-bis(methylene)-	114	C6H10O2	38
15.	Furan, 2,5-dimethyl-	96	C6H8O	38
16.	Cyclopentene, 1-ethyl-	96	C7H12	35
17.	Cyclopentene, 3-ethyl-	96	C7H12	35
18.	Cyclohexane, methylene-	96	C7H12	17
19.	1H-Pyrazole, 1,5-dimethyl-	96	C5H8N2	7
20.	Furan, 2,5-dimethyl-	96	C6H8O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	020521-42-0	576	48	58	2	108	6	53	0	44	9840
2.	*78	001120-73-6	593	50	47	1	77	7	46	0	39	9881
3.	*64	002758-18-1	594	50	47	1	56	17	37	4	39	8953
4.	*64	000000-00-0	591	37	67	2	61	20	37	0	39	9097
5.	*59	000627-19-0	116257	36	77	0	73	21	33	0	41	8704
6.	*56	013531-82-3	580	33	59	2	95	13	30	8	37	8425
7.	*50	000625-86-5	117590	45	62	2	61	33	25	11	38	5942
8.	45	000504-60-9	116263	45	56	1	79	24	19	0	35	7822
9.	45	000078-79-5	116269	40	50	1	82	21	19	2	31	7895
10.	*42	053566-37-3	606	39	81	1	61	30	17	0	35	7154
11.	*40	000625-86-5	117585	36	68	1	61	34	16	0	30	5806
12.	*39	000142-83-6	575	31	91	2	72	20	15	0	26	9247
13.	*39	029212-09-7	622	30	84	2	76	20	15	0	29	9540
14.	38	050521-50-1	2980	34	95	1	92	11	14	0	11	8966
15.	*38	000625-86-5	117586	33	77	2	67	36	14	0	35	5559
16.	*35	002146-38-5	635	52	37	3	90	51	11	19	41	8899
17.	*35	000694-35-9	117607	45	31	2	92	53	11	13	38	8569
18.	*17	001192-37-6	647	31	88	3	99	51	3	0	29	9169
19.	* 7	000694-31-5	560	30	43	1	48	80	1	0	27	5084
20.	* 7	000625-86-5	117584	29	67	1	60	78	1	0	26	5761

Peak 4



Scan 131 (7.248 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	708	57.90	65	82.00	72		
43.95	903	59.90	146	93.95	5687		
44.95	1992	60.75	153	94.95	273		
45.95	624	61.90	315	96.05	263		
47.95	1032	62.90	1110				
48.95	348	63.90	584				
49.80	115	64.90	550				
53.05	69	66.75	62				
54.95	138	76.80	74				
55.90	113	78.95	10000				
57.00	165	80.90	615				

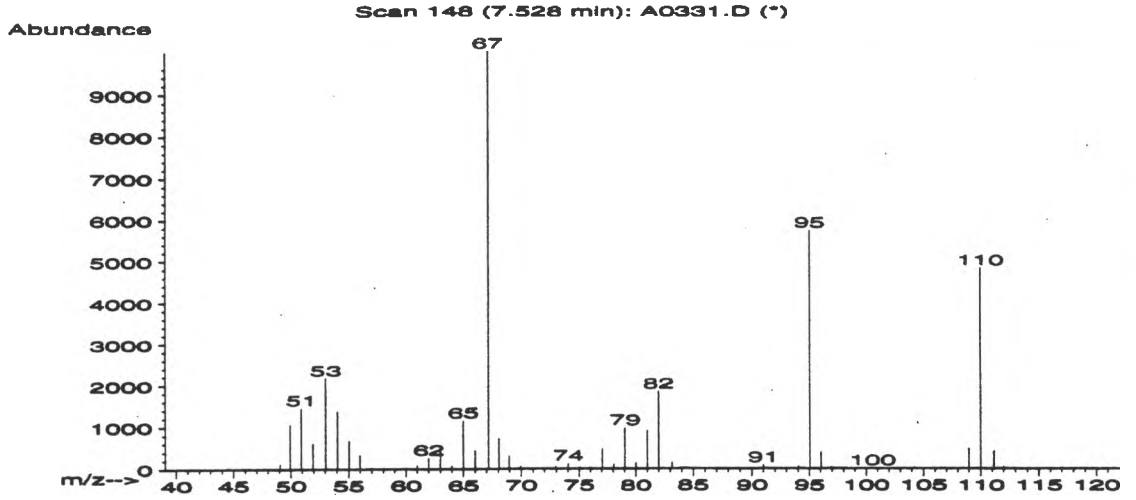
Scan 131 (7.248 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Methane, sulfonylbis-	94	C2H6O2S	86
2.	Methane, sulfonylbis-	94	C2H6O2S	74
3.	Methane, sulfonylbis-	94	C2H6O2S	72
4.	Methane, sulfonylbis-	94	C2H6O2S	72
5.	DIMETHYLPHOSPHINIC ACID	94	C2H7O2P	59
6.	Disulfide, dimethyl	94	C2H6S2	45
7.	Methane, sulfonylbis-	94	C2H6O2S	38
8.	Disulfide, dimethyl	94	C2H6S2	23
9.	Disulfide, dimethyl	94	C2H6S2	16
10.	Disulfide, dimethyl	94	C2H6S2	16
11.	Disulfide, dimethyl	94	C2H6S2	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	000067-71-0	117482	57	38	0	99	10	53	0	49	9902
2.	*74	000067-71-0	117480	59	40	1	87	17	44	0	56	9800
3.	*72	000067-71-0	117481	51	43	0	99	17	42	0	46	9779
4.	*72	000067-71-0	452	51	53	0	88	16	42	0	46	9852
5.	*59	000000-00-0	456	34	58	3	99	24	33	0	39	9748
6.	*45	000624-92-0	117489	36	68	2	85	22	19	5	32	7991
7.	*38	000067-71-0	117479	34	72	1	49	38	14	0	35	9626
8.	*23	000624-92-0	117488	39	52	1	38	46	6	1	27	7979
9.	*16	000624-92-0	117485	37	77	2	50	57	3	0	35	8134
10.	*16	000624-92-0	454	37	78	2	52	57	3	0	35	8121
11.	*12	000624-92-0	117484	32	68	2	38	57	2	0	26	7606

Peak 5



Scan 148 (7.528 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.05	122	63.00	449	75.95	21	94.05	49
49.95	1056	64.00	64	77.05	466	95.05	5734
50.95	1453	65.00	1143	78.05	107	96.05	389
51.95	605	66.00	439	79.05	970	96.95	39
53.05	2179	67.15	10000	80.00	139	100.55	7
54.05	1373	68.05	714	81.00	906	109.00	475
55.05	666	68.95	300	82.00	1846	110.00	4836
56.00	330	69.95	62	83.15	155	111.15	412
60.00	18	72.95	44	83.90	19	112.00	48
61.00	92	74.05	120	91.00	82		
62.00	262	75.05	26	92.05	16		

Compounds from Proctor and Gamble A0331.D

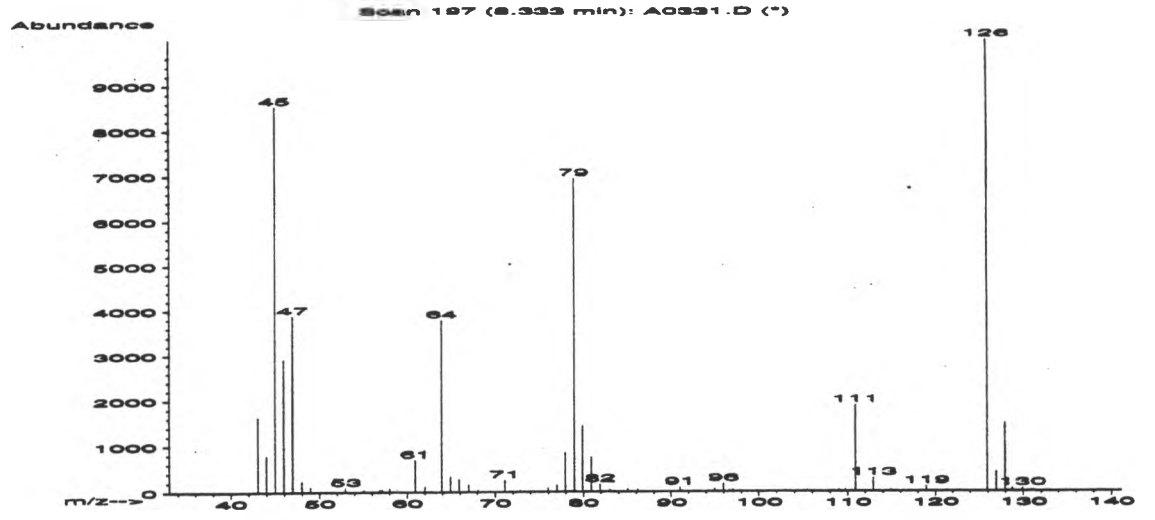
Scan 148 (7.528 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2,5-Dimethyl-2-cyclopentenone	110	C7H10O	80
2.	trans-4,5-Dimethylcyclopent-2-en-1-one	110	C7H10O	72
3.	TRANS-DIMETHYL-ISOPROPYLIDENE CYCLOPROPA	110	C8H14	53
4.	2,3-DIMETHYL-2-CYCLOPENTEN-1-ONE	110	C7H10O	53
5.	Pentalene, octahydro-, cis-	110	C8H14	53
6.	2,4-Hexadiene, 3,4-dimethyl-, (E,Z)-	110	C8H14	52
7.	3-Octyne	110	C8H14	47
8.	Cyclopropane, (1-methylethenyl)-	82	C6H10	43
9.	Cyclopropane, (1-methylethenyl)-	82	C6H10	43
10.	MENTHENE ISOMER B	138	C10H18	43
11.	Methyl-(endo-tricyclo[2.2.0.0(2,6)]hex-3	110	C7H10O	42
12.	2,4-Hexadiene	82	C6H10	41
13.	3-Hexyne	82	C6H10	38
14.	Cyclopropane, 1,2-dimethyl-3-methylene-	82	C6H10	38
15.	Cyclopentene, 1-methyl-	82	C6H10	35
16.	Bicyclo[3.1.0]hexane	82	C6H10	35
17.	1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	27
18.	2-Hexyne	82	C6H10	27
19.	1,3,7-Octatriene	108	C8H12	27
20.	Cyclopentene, 3-methyl-	82	C6H10	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000000-00-0	2189	49	28	1	99	15	48	0	46	9893
2.	*72	032556-65-3	2190	44	13	0	68	20	42	0	44	9693
3.	*53	000000-00-0	2262	46	59	2	78	28	28	12	38	9018
4.	*53	001121-05-7	2188	45	52	1	67	26	28	0	39	9329
5.	*53	001755-05-1	118910	44	51	2	88	28	28	17	38	7997
6.	*52	002417-88-1	2253	50	56	3	57	31	27	0	44	9100
7.	*47	015232-76-5	118878	33	56	2	45	36	20	0	39	8693
8.	*43	004663-22-3	116778	49	44	0	80	48	18	0	46	8085
9.	*43	004663-22-3	116777	47	52	0	83	48	18	0	44	8096
10.	43	029350-67-2	122308	47	33	0	39	44	18	0	39	8211
11.	*42	000000-00-0	2210	39	76	2	100	26	17	1	36	7258
12.	*41	000592-46-1	116773	69	14	0	78	51	16	17	58	7910
13.	*38	000928-49-4	116764	52	32	1	73	50	14	12	39	7227
14.	*38	062338-02-7	116779	49	46	1	99	55	14	0	44	8049
15.	*35	000693-89-0	116781	37	38	0	99	51	11	5	38	8033
16.	*35	000285-58-5	116792	36	55	1	89	51	11	0	39	8040
17.	*27	000931-36-2	118844	43	52	1	57	58	8	0	39	5226
18.	27	000764-35-2	116761	43	53	2	78	60	8	5	38	6588
19.	27	001002-35-3	1942	43	47	2	80	57	8	0	39	7859
20.	*25	001120-62-3	116783	32	40	0	99	52	7	4	37	7999

Peak 6



Scan 197 (8.333 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1639	58.00	77	75.95	77	91.00	90
43.95	790	60.90	687	76.95	144	94.95	56
44.95	8533	62.00	109	77.95	842	95.95	171
45.95	2905	63.90	3779	78.95	6915	96.70	35
46.95	3870	64.90	322	79.90	1436	97.05	32
47.95	233	65.90	273	80.90	754	105.40	35
48.95	104	67.00	154	81.90	159	108.40	16
52.95	87	68.05	37	83.00	39	109.00	41
55.05	41	71.05	246	83.50	29	109.75	34
56.90	50	71.95	14	85.00	60	110.90	1883
57.15	49	72.80	33	86.15	55	112.90	287

Scan 197 (8.333 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.90	30						
118.95	105						
125.95	10000						
126.95	419						
127.95	1490						
128.75	65						
129.90	59						
131.15	18						

Compounds from Proctor and Gamble A0331.D

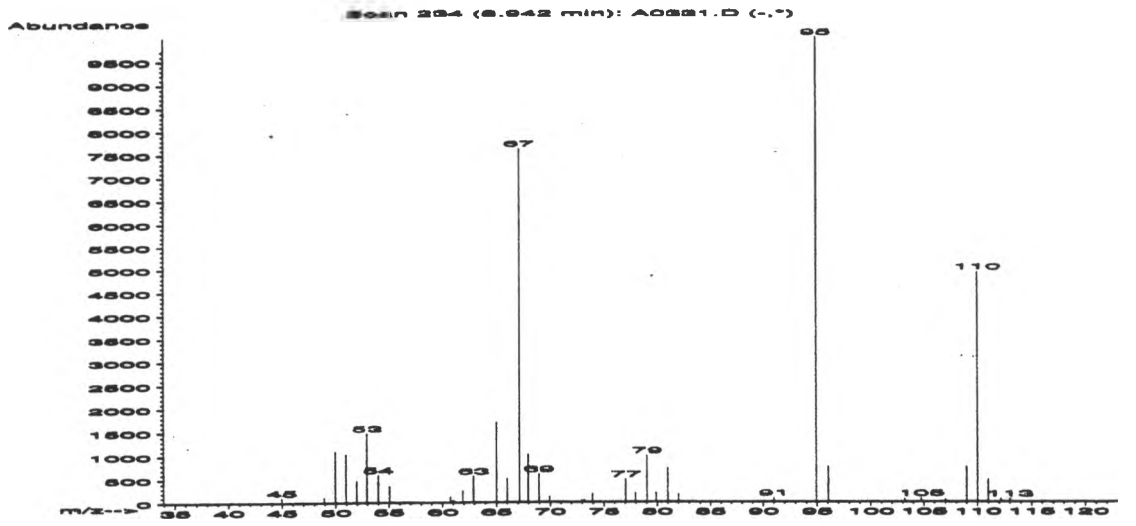
Scan 197 (8.333 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Trisulfide, dimethyl	126	C2H6S3	94
2.	Trisulfide, dimethyl	126	C2H6S3	91
3.	Trisulfide, dimethyl	126	C2H6S3	81
4.	S-METHYL METHYLTHIOSULPHONATE	126	C2H6O2S2	78
5.	Trisulfide, dimethyl	126	C2H6S3	74
6.	Trisulfide, dimethyl	126	C2H6S3	70
7.	Butane, 4-chloro-1,1,1-trifluoro-	146	C4H6ClF3	17
8.	METHYL ETHANE-2,2,2-D3-SULFONATE	124	C3H5D3O3S	12
9.	DIMETHYLDITHIOPHOSPHINIC ACID	126	C2H7PS2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	003658-80-8	120472	97	21	1	76	0	70	0	93	9928
2.	*91	003658-80-8	120469	77	44	2	88	0	62	0	74	9955
3.	*81	003658-80-8	120471	76	37	0	86	16	49	0	81	9843
4.	*78	002949-92-0	120465	36	9	0	99	10	46	5	38	7515
5.	*74	003658-80-8	5058	61	57	1	85	16	44	0	56	9844
6.	*70	003658-80-8	120470	69	40	1	99	27	41	0	68	8539
7.	17	000406-85-9	11122	34	85	0	83	53	3	0	25	7047
8.	*12	010307-06-9	4623	39	98	1	120	64	2	0	35	4298
9.	*10	016367-68-3	5060	39	67	2	80	66	1	0	35	6408

Peak 7



Scan 234 (8.942 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	7	61.90	250	77.05	498	107.00	52
44.95	109	62.90	565	77.95	192	109.00	754
48.90	112	65.00	1707	79.05	1000	110.00	4946
49.95	1099	66.00	512	79.90	198	111.00	487
50.95	1037	67.15	7591	81.00	731	112.15	71
51.95	467	67.95	1026	82.00	167	113.00	71
52.95	1482	68.95	612	91.00	87		
54.00	598	69.95	114	94.95	10000		
55.05	353	72.95	39	96.05	758		
60.75	117	73.20	48	103.20	63		
61.00	46	73.95	179	104.75	79		

Compounds from Proctor and Gamble A0331.D

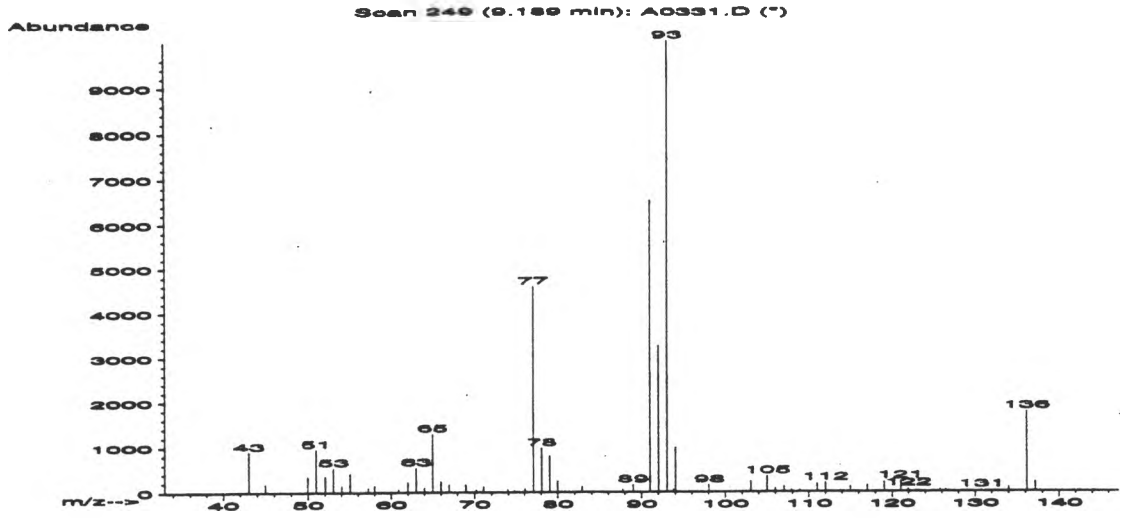
Scan 234 (8.942 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclobutene, 1,2,3,4-tetramethyl-, cis-	110	C8H14	83
2.	Cyclohexene, 1,2-dimethyl-	110	C8H14	78
3.	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	64
4.	2-Methyl-1-(methylamino)-1-cyanopropene	110	C6H10N2	53
5.	trans-4,5-Dimethylcyclopent-2-en-1-one	110	C7H10O	50
6.	2,3-DIMETHYL-2-CYCLOPENTEN-1-ONE	110	C7H10O	49
7.	4,5-Dimethyl-1,4-hexadiene	110	C8H14	47
8.	Ethanone, 1-(2-furanyl)-	110	C6H6O2	46
9.	Pentalene, octahydro-, cis-	110	C8H14	43
10.	3-Octyne	110	C8H14	43
11.	Ethanone, 1-(2-furanyl)-	110	C6H6O2	43
12.	Cyclopropane, 1,2-dimethyl-3-methylene-	82	C6H10	30
13.	3-Pyridinol	95	C5H5NO	27
14.	Pyridine N-oxide	95	C5H5NO	27
15.	Pyridine N-oxide	95	C5H5NO	27
16.	2,4-Hexadiene	82	C6H10	25
17.	Spirohexan-5-one	96	C6H8O	25
18.	1,4-Benzenediol	110	C6H6O2	15
19.	1H-Imidazole-2-carboxaldehyde, 1-methyl-	110	C5H6N2O	11
20.	1,3-Benzenediol	110	C6H6O2	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	002417-87-0	2265	34	9	0	68	1	50	0	41	8123
2.	*78	001674-10-8	2279	55	59	3	79	10	46	0	40	9695
3.	*64	000764-13-6	2251	58	51	1	72	24	37	0	46	9888
4.	*53	073171-64-9	2138	59	45	2	82	38	28	0	51	8665
5.	*50	032556-65-3	2190	36	21	0	78	32	25	0	41	9672
6.	*49	001121-05-7	2188	55	41	0	56	37	23	0	49	8003
7.	*47	000760-76-9	2244	36	21	1	74	40	20	0	41	9604
8.	*46	001192-62-7	118826	34	54	0	99	44	20	10	43	8377
9.	*43	001755-05-1	118910	50	45	2	60	42	18	19	41	5809
10.	*43	015232-76-5	118878	48	41	0	48	46	18	0	46	8933
11.	*43	001192-62-7	2127	33	44	0	99	45	18	0	41	8376
12.	*30	062338-02-7	116779	51	42	1	76	59	9	0	46	5665
13.	*27	000109-00-2	522	37	46	0	98	58	8	0	41	7598
14.	*27	000694-59-7	117536	43	51	3	90	56	8	0	40	7249
15.	*27	000694-59-7	519	48	30	1	70	60	8	16	41	7202
16.	*25	000592-46-1	116773	36	46	0	53	62	7	11	43	5481
17.	*25	020061-22-7	598	50	61	2	65	63	7	0	44	5224
18.	*15	000123-31-9	118840	61	30	1	54	77	2	0	56	4001
19.	*11	013750-81-7	118817	35	30	0	44	76	2	8	43	3960
20.	*11	000108-46-3	118837	45	47	1	54	76	2	0	44	4148

Peak 8



Scan 249 (9.189 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	899	62.00	222	76.05	78	94.05	980
44.95	177	63.00	536	77.05	4572	98.05	154
49.95	343	64.00	102	78.05	966	103.05	231
50.95	949	65.00	1287	79.05	794	105.00	342
52.05	362	66.00	230	80.00	239	106.00	69
53.05	536	67.00	163	82.90	122	107.00	123
54.05	146	68.95	163	87.75	55	107.90	41
55.05	419	70.20	48	89.00	158	108.90	35
57.25	94	71.05	117	91.00	6493	111.00	163
58.00	146	73.95	67	92.05	3249	112.00	196
60.90	64	74.80	30	93.05	10000	115.00	110

Scan 249 (9.189 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
117.05	138						
119.05	211						
121.05	232						
121.95	64						
122.80	19						
125.80	41						
126.45	36						
130.75	30						
134.00	86						
136.15	1758						
137.15	207						

CTMP 30.

Cmpd 11

Compounds from Proctor and Gamble A0331.D

Scan 249 (9.189 min): A0331.D

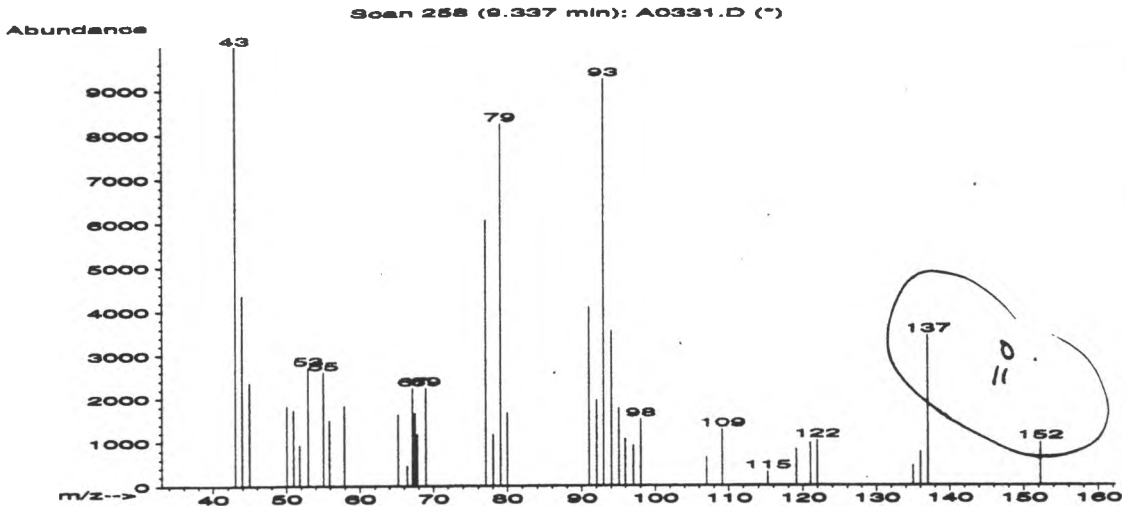
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-Phellandrene	136	C10H16	91
2.	.alpha.-Thujene	136	C10H16	91
3.	1-Phellandrene	136	C10H16	90
4.	1-Phellandrene	136	C10H16	90
5.	1-Phellandrene	136	C10H16	87
6.	1-Phellandrene	136	C10H16	87
7.	1-Phellandrene	136	C10H16	87
8.	.gamma.-Terpinene	136	C10H16	72
9.	Methylester of 1-Methyl-2,5-cyclohexadie	152	C9H12O2	64
10.	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-me	136	C10H16	64
11.	5,6-DIMETHYL-1,3-CYCLOHEXADIENE	108	C8H12	59
12.	.gamma.-Terpinene	136	C10H16	53
13.	.beta.-Phellandrene	136	C10H16	50
14.	Pyridine, 2-methyl-	93	C6H7N	50
15.	Pyridine, 2-methyl-	93	C6H7N	47
16.	Urea, phenyl-	136	C7H8N2O	46
17.	1-Phellandrene	136	C10H16	46
18.	Pyridine, 2-propyl-	121	C8H11N	43
19.	Pyridine, 2-propyl-	121	C8H11N	43
20.	.alpha.-Thujene	136	C10H16	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000099-83-2	121989	73	18	0	92	4	62	0	81	9713
2.	*91	002867-05-2	122055	69	26	1	93	3	60	17	50	9632
3.	*90	000099-83-2	121992	76	18	1	99	7	59	32	81	9481
4.	*90	000099-83-2	121991	77	15	0	71	7	59	15	66	9649
5.	*87	000099-83-2	121996	61	8	0	99	9	54	0	56	9857
6.	*87	000099-83-2	8088	68	23	1	99	12	54	0	76	9626
7.	*87	000099-83-2	121990	71	19	1	96	7	54	19	58	9487
8.	*72	000099-85-4	122004	46	56	3	96	11	42	12	40	9781
9.	64	059034-54-7	123931	44	5	0	94	16	37	0	39	9798
10.	*64	005794-03-6	8150	45	71	3	99	16	37	0	40	9717
11.	59	002417-81-4	1967	48	31	0	82	23	33	6	41	9497
12.	*53	000099-85-4	122009	46	48	3	86	29	28	5	40	8171
13.	*50	000555-10-2	122038	35	57	3	99	34	25	0	41	9250
14.	*50	000109-06-8	117455	36	56	2	99	34	25	0	41	7973
15.	*47	000109-06-8	117452	39	37	2	99	39	20	12	42	7889
16.	*46	000064-10-8	7775	35	43	2	88	44	20	2	43	7911
17.	*46	000099-83-2	121998	53	32	0	44	44	20	0	49	9726
18.	*43	000622-39-9	120065	33	37	1	99	43	18	0	41	7715
19.	*43	000622-39-9	120066	45	44	1	69	43	18	0	40	7737
20.	38	002867-05-2	8154	55	37	0	57	50	14	6	41	9727

Thujene organs in order of elution.

Peak 9



Scan 258 (9.337 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	10000	66.40	451	92.95	9237	121.95	1023
43.95	4354	67.15	2220	94.05	3539	135.00	442
44.95	2359	67.50	1648	95.05	1761	136.00	763
50.05	1821	67.80	1162	95.95	1058	137.00	3435
50.95	1717	68.95	2229	97.05	911	152.20	980
51.80	928	77.05	6036	98.05	1509		
52.95	2706	78.05	1171	107.00	642		
55.05	2593	79.05	8205	109.15	1275		
55.90	1483	80.00	1665	115.25	304		
57.90	1821	91.00	4076	119.05	824		
65.15	1613	92.05	1951	121.05	971		

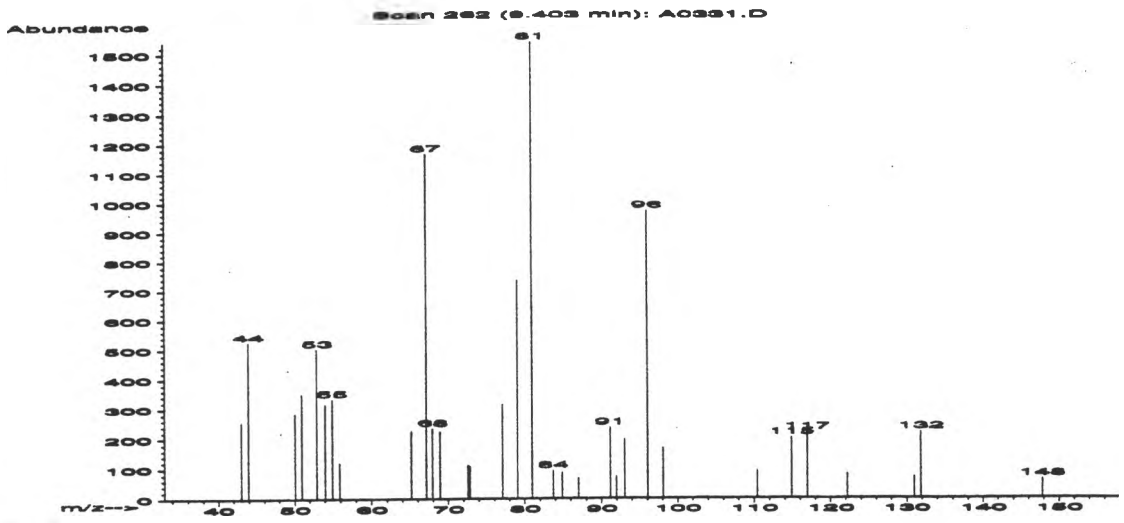
Scan 258 (9.337 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	exo-4-Methylbicyclo[3.2.1]octan-3-ene	122	C9H14	58
2.	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-me	136	C10H16	47
3.	3-CYCLOPROPYL-1,2-BUTADIENE	94	C7H10	38
4.	Trans-Ocimene	136	C10H16	38
5.	(+-)-trans-1-(1-Methylethenyl)-2-(2-meth	136	C10H16	38
6.	3-Oxatricyclo[3.2.1.0(2,4)]octane, (1.al	110	C7H10O	35
7.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	30
8.	1,3,5-Hexatriene, 2-methyl-	94	C7H10	30
9.	1,3,5-Hexatriene, 3-methyl-, (E)-	94	C7H10	30
10.	Bicyclo[3.1.0]hex-3-en-2-one, 5-(1-methy	136	C9H12O	30
11.	1,3,5-Hexatriene, 3-methyl-, (Z)-	94	C7H10	30
12.	.BETA.-OCIMENE-X	136	C10H16	27
13.	.ALPHA.-PINENE, (-)-	136	C10H16	27
14.	(1-Butylidene)cyclohexane	136	C10H16	27
15.	Sabinene	136	C10H16	27
16.	Benzenamine, 2-methyl-5-nitro-	152	C7H8N2O2	25
17.	.beta.-Phellandrene	136	C10H16	25
18.	3-Undecen-5-yne, (Z)-	150	C11H18	22
19.	.beta.-Myrcene	136	C10H16	22
20.	.ALPHA.-PINENE, (-)-	136	C10H16	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	078965-86-3	4484	49	48	1	78	27	32	6	47	8403
2.	*47	005794-03-6	8150	45	69	2	83	38	20	0	40	8902
3.	*38	000000-00-0	492	37	52	0	72	54	14	23	43	7414
4.	*38	000502-99-8	8063	36	81	2	92	50	14	0	39	8699
5.	*38	080082-35-5	8076	35	57	2	92	46	14	0	39	8618
6.	35	003146-39-2	2209	68	58	0	59	55	11	0	42	6688
7.	*30	003779-61-1	121952	52	63	1	67	58	9	0	44	8620
8.	*30	019264-50-7	487	44	53	0	68	57	9	0	44	7501
9.	*30	024587-26-6	489	44	59	0	77	57	9	0	44	7427
10.	*30	036262-12-1	7993	53	61	2	63	58	9	0	49	7791
11.	*30	024587-27-7	488	44	54	0	76	57	9	0	44	7491
12.	*27	013877-91-3	121957	35	66	3	254	58	8	0	39	7493
13.	*27	000080-56-8	122067	43	59	0	54	59	8	13	40	8105
14.	*27	036144-40-8	8123	34	67	2	82	58	8	18	40	8164
15.	*27	003387-41-5	122063	43	58	0	63	58	8	5	40	7729
16.	*25	000099-55-8	123856	36	35	0	53	65	7	10	43	6573
17.	*25	000555-10-2	122039	60	45	2	131	61	7	24	46	8188
18.	22	074744-27-7	12908	43	60	0	57	61	5	2	41	8590
19.	*22	000123-35-3	121967	34	65	1	72	65	5	5	40	7787
20.	*22	000080-56-8	122070	36	59	0	64	65	5	0	41	7474

Peak 10



Scan 262 (9.403 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	255	68.95	223	93.05	197		
43.95	524	72.55	111	96.05	971		
50.05	283	72.80	107	98.05	169		
50.95	348	77.05	313	110.40	92		
52.95	501	79.05	737	114.90	202		
54.05	314	81.00	1540	116.95	220		
54.95	332	83.75	93	122.20	82		
55.90	119	84.90	87	131.00	72		
65.15	224	87.00	68	131.90	222		
67.15	1161	91.15	236	147.80	63		
67.95	233	91.95	72				

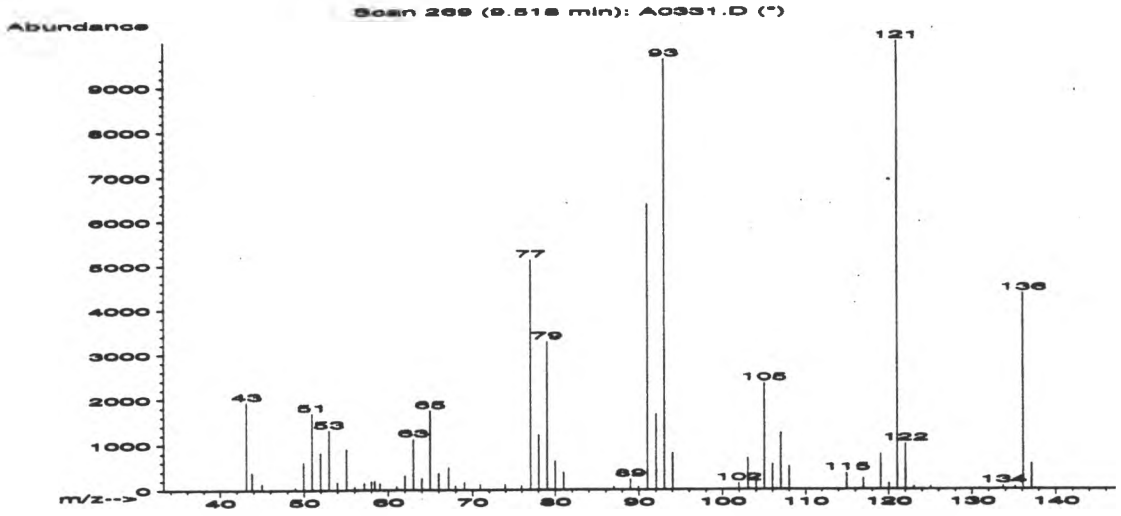
Scan 262 (9.403 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2,3-Hexadiene, 2-methyl-	96	C7H12	72
2.	3,4-Heptadiene	96	C7H12	64
3.	2,4-Hexadiene, 1-chloro-	116	C6H9Cl	53
4.	1,3-PENTADIENE, 2,3-DIMETHYL-	96	C7H12	47
5.	1,4-Heptadiene, 3-methyl-	110	C8H14	40
6.	METHYLENECYCLOOCTANE	124	C9H16	38
7.	2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	35
8.	2,4-Hexadienal, (E,E)-	96	C6H8O	32
9.	Cyclopentene, 4,4-dimethyl-	96	C7H12	27
10.	2,4-Hexadiene, 3-methyl-	96	C7H12	27
11.	1,4-Hexadiene, 5-methyl-	96	C7H12	25
12.	2,4-Hexadiene, 2-methyl-	96	C7H12	25
13.	2,5-Heptadiene, (E,E)-	96	C7H12	25
14.	1,4-Hexadiene, 2-methyl-	96	C7H12	25
15.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	23
16.	1,4-Hexadiene, 4-methyl-	96	C7H12	17
17.	2,4-Heptadiene, (E,E)-	96	C7H12	16
18.	2,4-Hexadiene, 2-methyl-	96	C7H12	16
19.	3-Heptyne	96	C7H12	16
20.	CYCLOBUTANE, ISOPROPYLIDEN-	96	C7H12	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	029212-09-7	622	58	41	0	87	12	42	10	41	9715
2.	*64	002454-31-1	615	54	49	0	95	18	37	5	38	9692
3.	53	034632-89-8	3395	45	53	0	99	27	28	8	41	8831
4.	*47	000000-00-0	626	34	70	0	99	36	20	0	41	9124
5.	40	001603-01-6	2229	39	63	1	87	32	16	14	34	8965
6.	38	003618-18-6	4932	42	82	2	99	21	14	0	29	9680
7.	*35	001120-73-6	593	37	59	0	53	55	11	0	41	6926
8.	*32	004488-48-6	574	32	72	0	99	50	9	0	33	8837
9.	*27	019037-72-0	638	37	58	2	252	57	8	0	39	8369
10.	*27	028823-42-9	624	34	68	2	158	57	8	0	39	9073
11.	*25	000763-88-2	619	37	59	1	153	51	7	11	37	9038
12.	*25	028823-41-8	117606	39	56	1	148	54	7	5	34	9001
13.	*25	039619-60-8	614	36	58	1	134	54	7	11	37	9101
14.	*25	001119-14-8	617	37	59	1	150	51	7	4	37	9154
15.	23	002758-18-1	117591	41	75	3	147	48	6	0	29	7971
16.	*17	001116-90-1	618	30	64	1	155	54	3	3	29	9122
17.	*16	002384-94-3	613	33	63	2	144	60	3	6	35	9063
18.	*16	028823-41-8	623	28	74	2	163	57	3	5	34	9116
19.	*16	002586-89-2	603	34	71	1	60	57	3	7	37	9211
20.	*12	000000-00-0	633	31	65	2	288	63	2	1	30	8299

Peak 11



Scan 269 (9.518 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.15	1932	57.15	152	67.95	93	89.00	245
43.80	382	58.00	192	69.05	172	89.90	70
44.95	137	58.40	193	70.95	121	91.00	6373
48.95	56	59.00	142	73.95	121	92.05	1665
49.95	609	61.00	79	75.95	97	93.05	9599
50.95	1685	62.00	326	77.05	5128	94.05	808
51.95	816	63.00	1118	78.05	1217	101.95	144
52.95	1312	64.00	259	79.05	3287	103.05	693
53.95	169	65.00	1746	80.00	642	104.00	282
55.05	904	66.00	370	81.00	386	105.00	2354
56.00	72	67.15	504	87.00	75	106.00	563

Scan 269 (9.518 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	1242	125.05	62				
108.00	505	133.75	78				
110.00	24	135.15	58				
110.50	21	136.15	4367				
115.00	365	137.15	569				
116.95	242						
119.05	775						
120.05	134						
121.05	10000						
122.05	1014						
123.05	63						

CTMP 31
CPMD 12

Compounds from Proctor and Gamble A0331.D

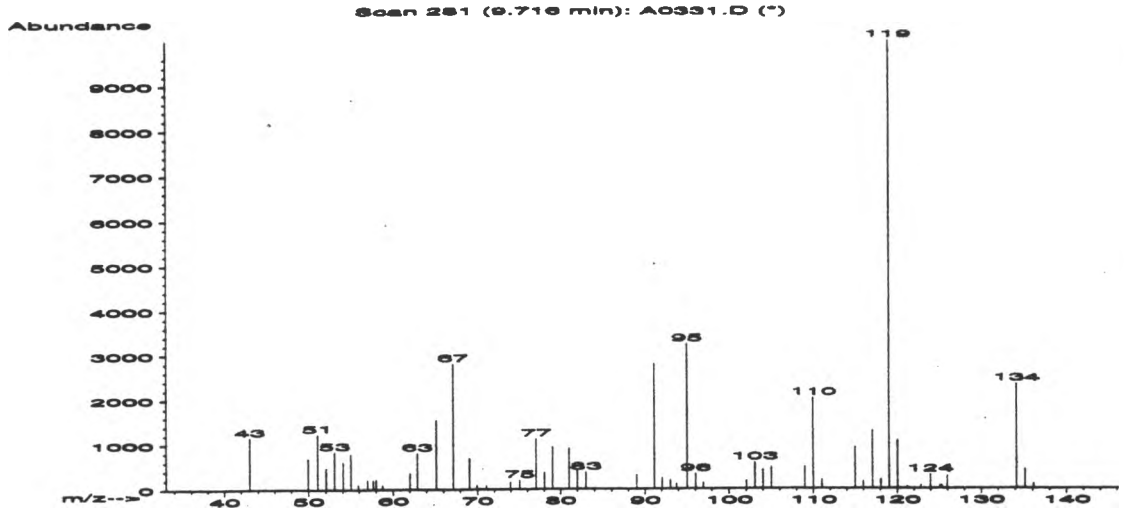
Scan 269 (9.518 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	.alpha.-Terpinene	136	C10H16	96
2.	.alpha.-Terpinene	136	C10H16	96
3.	.alpha.-Terpinene	136	C10H16	95
4.	.alpha.-Terpinene	136	C10H16	93
5.	.DELTA.-4-CARENE	136	C10H16	93
6.	.ALPHA.-TERPINOLENE	136	C10H16	93
7.	.ALPHA.-TERPINOLENE	136	C10H16	93
8.	Isoterpinolene	136	C10H16	93
9.	.alpha.-Terpinene	136	C10H16	90
10.	.ALPHA.-TERPINOLENE	136	C10H16	90
11.	.alpha.-Terpinene	136	C10H16	90
12.	Benzenemethanol, .alpha.,4-dimethyl-	136	C9H12O	87
13.	Bornylene	136	C10H16	87
14.	.ALPHA.-TERPINOLENE	136	C10H16	64
15.	1,3,6-OCTATRIENE, 3,7-DIMETHYL-	136	C10H16	64
16.	.ALPHA.-TERPINOLENE	136	C10H16	64
17.	Alloocimene	136	C10H16	64
18.	cis-Ocimene	136	C10H16	55
19.	.ALPHA.-TERPINOLENE	136	C10H16	55
20.	.ALPHA.-TERPINOLENE	136	C10H16	55

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000099-86-5	121987	106	7	0	77	3	76	16	96	9923
2.	*96	000099-86-5	8087	97	16	0	95	6	76	0	96	9929
3.	*95	000099-86-5	121985	89	23	0	87	9	74	0	95	9892
4.	*93	000099-86-5	121981	80	32	0	83	6	66	0	93	9926
5.	*93	000554-61-0	122087	80	30	0	87	6	66	0	93	9885
6.	*93	000586-62-9	122030	86	20	1	88	9	66	47	93	9747
7.	*93	000586-62-9	122034	83	26	1	86	9	66	46	90	9741
8.	*93	000586-63-0	8112	87	23	1	90	9	66	0	91	9778
9.	*90	000099-86-5	121986	76	36	2	96	9	59	0	81	9840
10.	*90	000586-62-9	122035	83	29	1	85	9	59	17	66	9741
11.	*90	000099-86-5	121983	76	19	0	98	6	59	2	66	9846
12.	*87	000536-50-5	121918	74	33	2	90	15	54	17	66	9499
13.	*87	000464-17-5	8146	69	47	2	85	9	54	5	52	9823
14.	*64	000586-62-9	122032	73	34	0	67	31	37	20	66	9798
15.	*64	000000-00-0	8059	71	37	1	98	33	37	0	68	8654
16.	*64	000586-62-9	8113	67	50	0	64	33	37	0	64	9679
17.	*64	000673-84-7	121964	77	29	1	98	33	37	0	81	8594
18.	*55	029714-87-2	121959	82	38	1	53	44	29	35	74	9658
19.	*55	000586-62-9	122033	66	42	0	45	44	29	0	64	9702
20.	*55	000586-62-9	122031	65	54	0	57	44	29	0	64	9819

Peak 12



Scan 281 (9.716 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1162	58.75	91	78.05	361	96.05	334
49.95	693	62.00	356	79.05	938	96.95	134
51.05	1234	62.90	811	81.00	911	102.05	174
52.05	469	65.15	1549	82.00	419	103.05	591
53.05	840	67.15	2803	83.00	379	104.00	429
54.05	606	69.05	696	89.00	316	105.00	479
54.95	786	69.95	93	91.15	2799	109.00	492
55.90	108	71.05	81	92.05	240	110.00	2035
57.00	200	73.95	155	93.05	202	111.00	199
57.65	197	75.05	199	93.80	108	115.00	929
58.00	213	77.05	1122	95.05	3250	116.00	160

Scan 281 (9.716 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
117.05	1302	135.15	430				
118.05	205	136.15	101				
119.05	10000						
120.05	1075						
121.20	47						
122.80	75						
123.95	315						
125.05	70						
125.30	70						
125.95	280						
134.15	2346						

CTMP 32

CPMD 013

Scan 281 (9.716 min): A0331.D

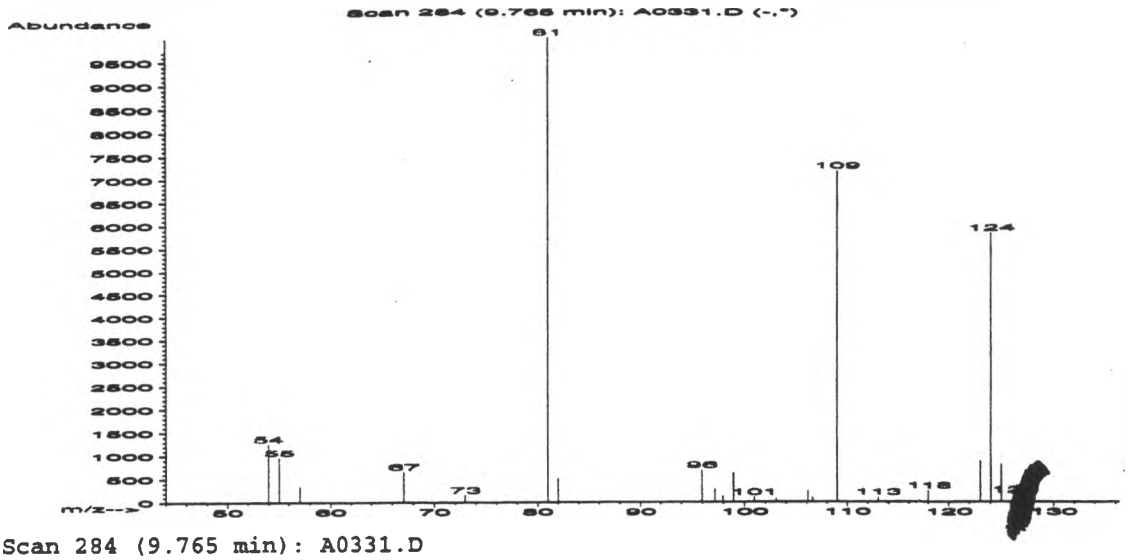
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	91
2.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	91
3.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	91
4.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	91
5.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	83
6.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	76
7.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	64
8.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	64
9.	Benzene, 1-methyl-2-(1-methylethyl)-	134	C10H14	64
10.	Benzene, methyl(1-methylethyl)-	134	C10H14	64
11.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	64
12.	Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	64
13.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	64
14.	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	64
15.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	64
16.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	64
17.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	64
18.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	64
19.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	60
20.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	58

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000527-84-4	7445	82	7	0	99	32	60	0	93	9073
2.	*91	000527-84-4	121625	82	6	0	88	32	60	0	93	9079
3.	*91	000099-87-6	121631	81	7	0	98	32	60	0	93	9068
4.	*91	000535-77-3	121630	81	11	0	92	32	60	0	93	9088
5.	*83	000099-87-6	121639	88	6	1	86	32	50	1	91	9077
6.	*76	000933-98-2	121653	73	17	1	96	25	45	40	76	9040
7.	*64	000099-87-6	121632	77	14	1	97	32	37	30	76	9036
8.	*64	000535-77-3	7446	72	17	0	93	35	37	0	76	9065
9.	*64	000527-84-4	121624	77	15	1	99	32	37	0	81	9073
10.	*64	025155-15-1	121626	79	11	1	79	35	37	10	74	9080
11.	*64	000099-87-6	121633	80	10	0	82	35	37	25	81	9077
12.	*64	000934-74-7	121668	74	19	1	84	32	37	35	76	9042
13.	*64	000535-77-3	121627	74	15	1	87	35	37	12	76	9074
14.	*64	000095-93-2	121674	68	24	1	98	32	37	41	70	8633
15.	*64	000535-77-3	121628	73	16	1	93	31	37	0	76	9120
16.	*64	000099-87-6	121635	76	12	0	78	32	37	0	81	9077
17.	*64	000535-77-3	121629	77	12	0	87	32	37	0	81	9071
18.	*64	002870-04-4	7454	67	22	1	87	35	37	23	64	9052
19.	*60	000933-98-2	121654	64	27	1	84	37	35	0	64	9028
20.	*58	000099-87-6	121636	69	21	1	94	32	32	2	58	9075

Peak 13

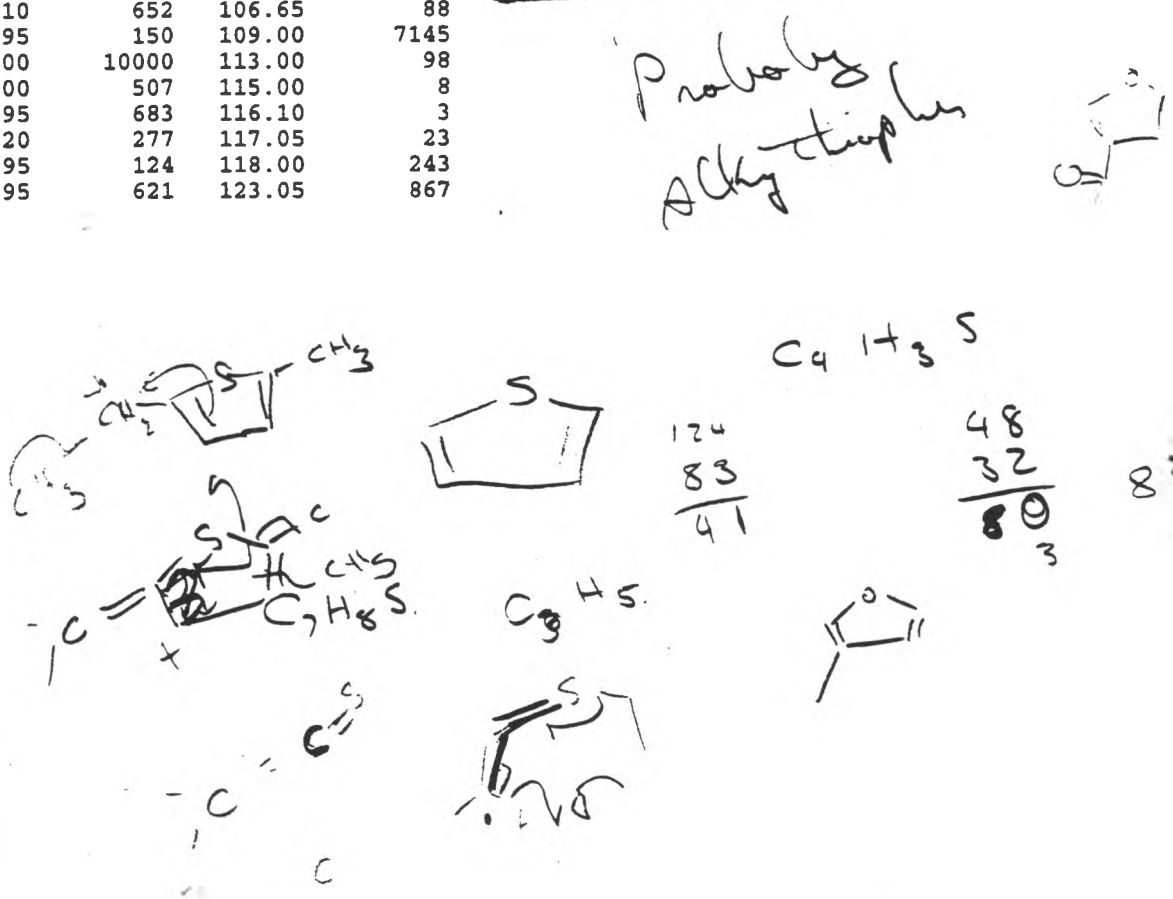
required subtraction from both sides



Scan 284 (9.765 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
54.00	1253	100.95	104	124.05	5792		
55.05	960	103.05	65	125.05	802		
57.05	329	106.15	236	[redacted]	150		
67.10	652	106.65	88				
72.95	150	109.00	7145				
81.00	10000	113.00	98				
82.00	507	115.00	8				
95.95	683	116.10	3				
97.20	277	117.05	23				
97.95	124	118.00	243				
98.95	621	123.05	867				



Compounds from Proctor and Gamble A0331.D

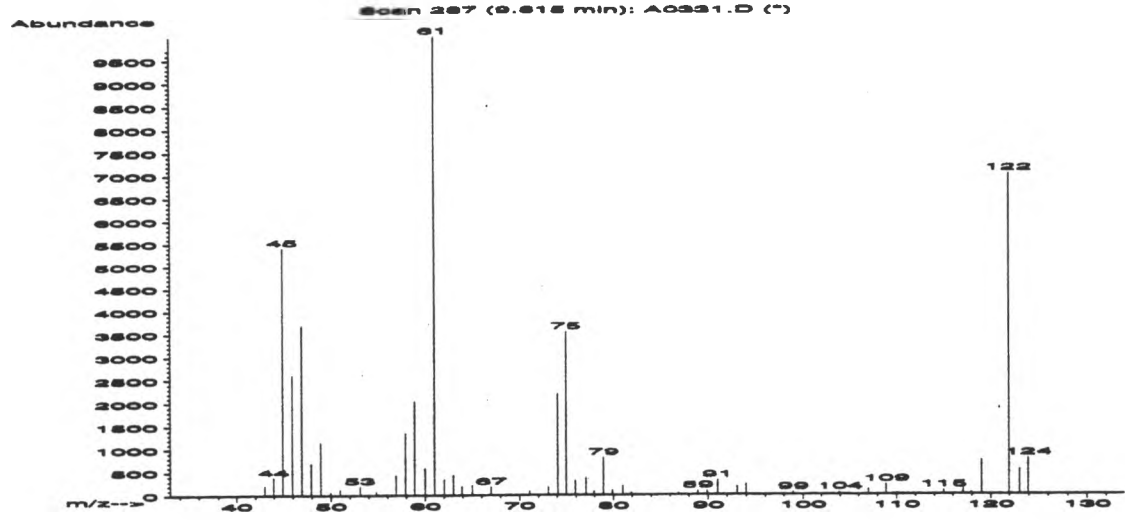
Scan 284 (9.765 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-methoxy-	124	C7H8O2	80
2.	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	72
3.	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	72
4.	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	72
5.	2-Cyclopenten-1-one, 3,4,4-trimethyl-	124	C8H12O	56
6.	Cycloopent-2-ene-1-one, 2,3,4-trimethyl-	124	C8H12O	53
7.	Ethanone, 1-(2-methyl-1-cyclopenten-1-yl	124	C8H12O	50
8.	Phenol, 2-methoxy-	124	C7H8O2	50
9.	2-Cyclopenten-1-one, 2,3,4-trimethyl-	124	C8H12O	43
10.	3-Acetyl-1-cyclohexene	124	C8H12O	42
11.	Bicyclo[3.3.1]nonane	124	C9H16	33
12.	Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	32
13.	Phenol, 2-methoxy-	124	C7H8O2	32
14.	Phenol, 4-methoxy-	124	C7H8O2	25
15.	Phenol, 2-methoxy-	124	C7H8O2	25
16.	1,4-Pentadiene, 3,3-dimethyl-	96	C7H12	25
17.	2-(1-METHYLVINYL)THIOPHENE	124	C7H8S	12
18.	4,5-DIMETHYL-2-PYRIMIDONE	124	C6H8N2O	12
19.	2-Cyclopenten-1-one, 3,4,5-trimethyl-	124	C8H12O	10
20.	2-AMINO-6-METHYL-3-PYRIDINOL	124	C6H8N2O	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000090-05-1	120381	34	52	0	86	15	48	2	43	9905
2.	*72	000932-66-1	120413	38	67	1	99	15	42	0	39	9846
3.	*72	000932-66-1	120412	38	64	0	96	12	42	0	39	9898
4.	*72	000932-66-1	4805	38	64	1	99	12	42	0	39	9926
5.	*56	030434-65-2	4785	44	53	1	85	11	30	7	36	8890
6.	*53	083321-16-8	4858	35	59	2	140	29	28	0	41	9033
7.	*50	003168-90-9	4790	33	69	0	81	35	25	0	41	8371
8.	*50	000090-05-1	120380	28	55	0	76	16	25	2	35	9868
9.	*43	028790-86-5	4783	43	57	1	63	43	18	0	39	9337
10.	*42	000000-00-0	4806	29	66	0	68	29	17	2	35	9054
11.	*33	000280-65-9	120445	29	89	2	77	35	10	0	29	7979
12.	*32	000932-66-1	120414	30	70	0	63	48	9	0	33	9881
13.	*32	000090-05-1	120376	30	71	0	71	48	9	0	33	9339
14.	*25	000150-76-5	120386	30	62	0	65	52	7	0	33	8922
15.	*25	000090-05-1	120383	29	62	0	71	51	7	0	33	9384
16.	*25	001112-35-2	628	29	58	0	69	51	7	0	33	7347
17.	*12	030616-73-0	4734	30	67	2	57	56	2	2	29	6606
18.	*12	034939-17-8	4681	35	69	1	50	64	2	0	35	5311
19.	*10	055683-21-1	4786	33	55	1	97	70	1	0	35	8609
20.	* 9	000000-00-0	4677	28	59	0	56	71	1	0	33	4324

Peak 14



Scan 287 (9.815 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	197	56.90	433	73.05	174	86.90	34
43.95	380	57.90	1342	74.05	2198	88.90	85
44.95	5402	58.90	2033	74.95	3549	89.90	81
45.95	2599	60.00	576	75.95	302	91.00	320
46.95	3681	61.00	10000	77.05	378	93.05	177
47.95	692	62.00	344	77.95	81	93.95	227
48.95	1141	63.00	438	78.95	811	96.95	23
49.95	64	63.90	193	79.90	102	98.95	48
50.95	133	65.00	228	81.00	201	103.95	50
53.05	188	67.00	174	81.90	55	107.00	114
54.80	69	71.05	84	84.75	17	108.90	217

Scan 287 (9.815 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.00	35						
115.00	89						
117.05	116						
117.95	40						
119.05	741						
121.05	23						
121.95	7010						
123.05	553						
123.95	784						

Compounds from Proctor and Gamble A0331.D

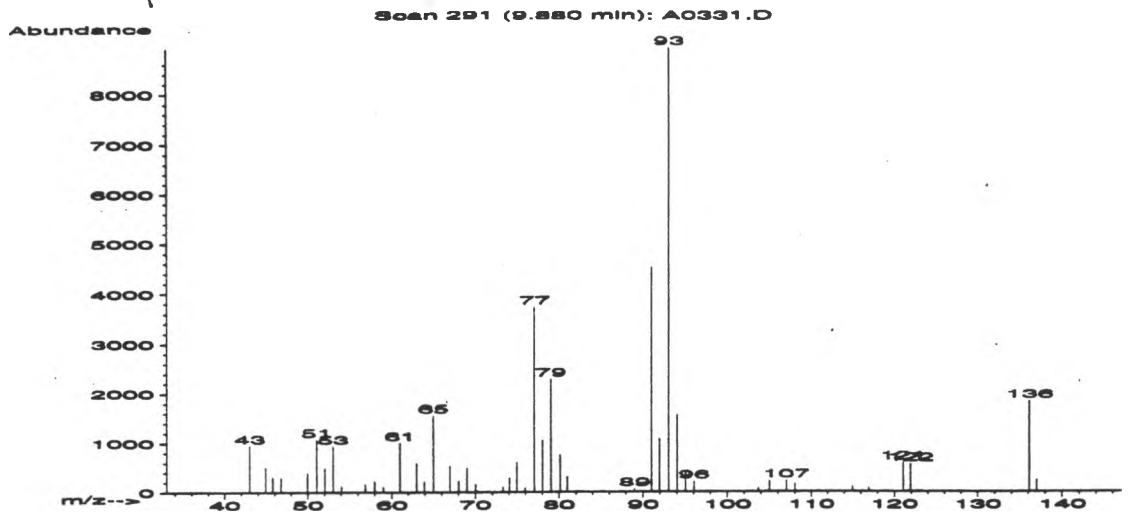
Scan 287 (9.815 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethane, 1,2-bis(methylthio)-	122	C4H10S2	94
2.	Ethane, 1,2-bis(methylthio)-	122	C4H10S2	87
3.	Tungsten, [1,2-bis(methylthio)ethane-S,S	418	C8H10O4S2W	74
4.	Ethane, 1,2-bis(methylthio)-	122	C4H10S2	72
5.	2-(METHYLTHIO)ETHANOL	92	C3H8OS	38
6.	Ethanol, 2,2'-thiobis-	122	C4H10O2S	28
7.	Propanoic acid, 3-(methylthio)-	120	C4H8O2S	28
8.	Ethanol, 2,2'-thiobis-	122	C4H10O2S	28
9.	Hydrazinecarbodithioic acid, methyl este	122	C2H6N2S2	22
10.	[2,4-13C]-1,3-Dithiane	120	C313CH8S2	16
11.	2,4,6-Cycloheptatrien-1-one, 2-hydroxy-	122	C7H6O2	10
12.	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	9
13.	Hydrazinecarbodithioic acid, methyl este	122	C2H6N2S2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	006628-18-8	120142	92	19	1	96	3	70	7	83	9776
2.	*87	006628-18-8	4299	77	46	0	84	14	54	10	66	9623
3.	74	038536-75-3	100652	38	89	0	93	0	44	0	33	8658
4.	*72	006628-18-8	120143	40	4	0	76	12	42	0	39	8464
5.	38	005271-38-5	117413	46	67	2	99	36	14	0	34	8268
6.	28	000111-48-8	120127	34	88	2	67	40	8	0	22	8401
7.	28	000646-01-5	119939	54	66	2	54	38	8	8	28	7801
8.	28	000111-48-8	120131	41	49	2	88	40	8	0	28	8276
9.	*22	005397-03-5	4262	34	73	2	70	62	5	0	39	6482
10.	16	000000-00-0	4045	45	62	1	68	58	3	11	33	6733
11.	*10	000533-75-5	4339	47	41	1	63	75	1	9	38	5066
12.	9	000111-77-3	119961	44	30	2	39	76	1	4	37	4000
13.	7	005397-03-5	120109	36	96	3	86	63	1	0	18	7120

Peak 15 β-Phellandrene.



Scan 291 (9.880 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	941	59.00	102	74.95	602	94.05	1555
44.95	501	61.00	997	75.95	81	95.05	421
45.80	299	63.00	582	77.05	3703	96.05	207
46.80	290	63.90	214	78.05	1046	103.70	70
49.95	385	65.00	1551	79.05	2272	105.00	213
51.05	1065	67.00	527	80.15	751	107.00	217
52.05	488	68.05	222	81.00	304	108.00	159
53.05	928	69.05	487	89.00	56	115.00	94
54.05	116	70.05	155	91.00	4501	116.95	71
56.90	160	73.30	103	91.95	1076	121.05	586
58.00	223	74.05	286	93.05	8910	121.95	550

Scan 291 (9.880 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
136.15	1824						
137.00	240						

CTMP. 033
Cmpd. 05

Compounds from Proctor and Gamble A0331.D

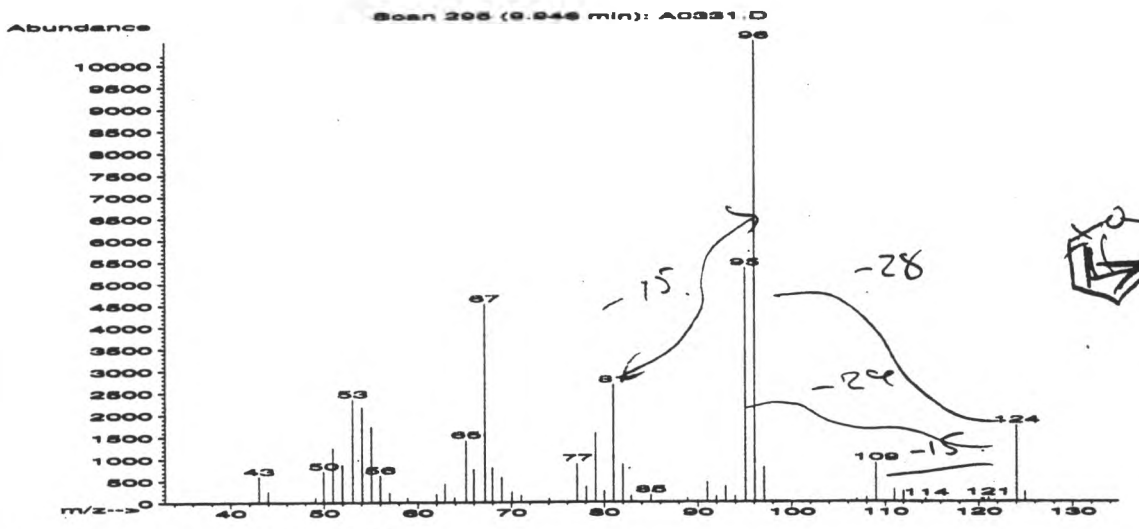
Scan 291 (9.880 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Sabinene	136	C10H16	90
2.	Sabinene	136	C10H16	87
3.	.beta.-Phellandrene	136	C10H16	87
4.	Sabinene	136	C10H16	86
5.	.beta.-Phellandrene	136	C10H16	83
6.	(-)-.BETA.-PINENE	136	C10H16	72
7.	Sabinene	136	C10H16	72
8.	.gamma.-Terpinene	136	C10H16	72
9.	.beta.-Thujene	136	C10H16	68
10.	1-Phellandrene	136	C10H16	64
11.	Sabinene	136	C10H16	64
12.	BICYCLO[2.2.1]HEPT-2-ENE, 2,7,7-TRIMETHY	136	C10H16	64
13.	1-Phellandrene	136	C10H16	59
14.	TRICYCLO[2.2.1.0(2,6)]HEPTANE, 2,3,3-TRI	136	C10H16	59
15.	1-Phellandrene	136	C10H16	59
16.	1-Phellandrene	136	C10H16	59
17.	.DELTA.3-Carene	136	C10H16	59
18.	.beta.-Phellandrene	136	C10H16	52
19.	1-Phellandrene	136	C10H16	50
20.	.beta.-Phellandrene	136	C10H16	45

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	003387-41-5	122063	69	31	1	87	9	59	20	70	9814
2.	*87	003387-41-5	122064	68	31	2	91	9	54	22	58	9853
3.	*87	000555-10-2	122038	68	28	2	99	8	54	12	58	9833
4.	*86	003387-41-5	122060	52	49	2	99	10	53	0	44	9862
5.	*83	000555-10-2	122040	62	18	1	90	12	50	0	56	9910
6.	*72	000000-00-0	8164	57	49	2	99	18	42	0	49	9727
7.	*72	003387-41-5	122061	53	31	0	66	17	42	0	49	9758
8.	*72	000099-85-4	122004	51	56	2	76	19	42	0	46	9717
9.	*68	028634-89-1	8155	61	31	1	99	24	40	0	56	9810
10.	*64	000099-83-2	121989	50	41	1	99	23	37	0	46	9656
11.	64	003387-41-5	122059	58	40	1	93	17	37	0	39	9824
12.	*64	000000-00-0	8147	56	53	2	79	19	37	0	40	9157
13.	*59	000099-83-2	121991	48	46	2	88	25	33	0	39	9619
14.	*59	000000-00-0	8189	43	65	3	99	25	33	0	40	9573
15.	*59	000099-83-2	121996	47	22	1	99	24	33	0	40	9593
16.	*59	000099-83-2	121992	35	61	2	90	25	33	13	40	9569
17.	*59	013466-78-9	122095	33	68	3	99	25	33	1	40	9669
18.	*52	000555-10-2	122041	51	41	1	85	31	27	0	46	9523
19.	*50	000099-83-2	121993	36	53	2	91	35	25	1	40	9561
20.	*45	000555-10-2	8118	61	34	3	138	48	19	0	56	9815

Peak 16

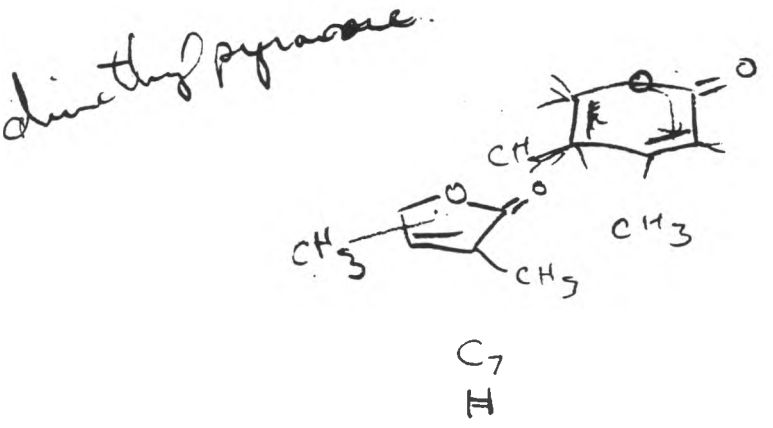


Scan 295 (9.946 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	595	58.90	104	74.05	88	91.95	126
43.95	249	62.00	186	77.05	882	92.95	360
49.05	111	62.90	428	78.05	356	93.95	137
49.95	711	63.90	117	79.05	1577	95.05	5349
50.95	1246	65.15	1410	80.00	253	96.05	10533
51.95	861	66.00	758	81.00	2667	97.05	799
53.05	2341	67.15	4525	82.00	868	106.90	64
54.05	2170	67.95	797	82.90	152	108.00	90
55.05	1721	68.95	580	85.00	163	109.00	887
56.00	618	70.05	231	88.90	82	111.00	281
57.00	216	71.05	158	91.00	457	112.00	238

Scan 295 (9.946 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
114.40	77						
120.30	75						
120.55	77						
121.05	89						
121.70	34						
124.05	1741						
124.95	222						



Compounds from Proctor and Gamble A0331.D

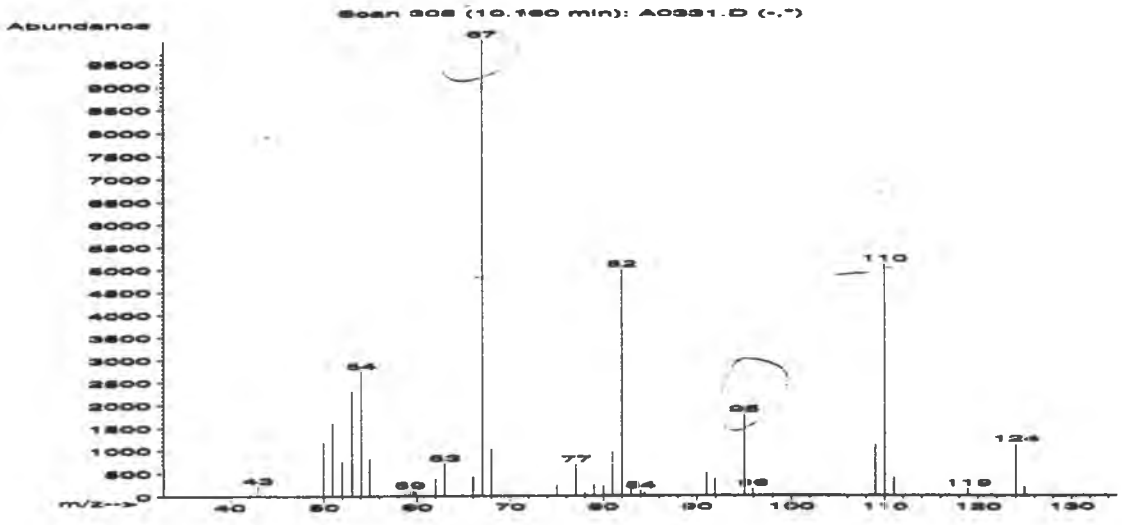
Scan 295 (9.946 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2,4-Hexadienal	96	C6H8O	64
2.	1-Pyrrolidinecarbonitrile	96	C5H8N2	47
3.	1H-Imidazole, 1,2-dimethyl-	96	C5H8N2	43
4.	2-Butenal, 2-ethenyl-	96	C6H8O	42
5.	Pyrazole, 1,4-dimethyl-	96	C5H8N2	38
6.	1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	38
7.	1H-Imidazole, 2,4-dimethyl-	96	C5H8N2	37
8.	1H-Pyrazole, 3,5-dimethyl-	96	C5H8N2	35
9.	1H-Pyrazole, 3,5-dimethyl-	96	C5H8N2	35
10.	2-Nonyne	124	C9H16	32
11.	3,5-Octadien-2-one, (E,E)-	124	C8H12O	30
12.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	25
13.	1H-Pyrazole, 3,5-dimethyl-	96	C5H8N2	25
14.	1H-Pyrazole, 3,5-dimethyl-	96	C5H8N2	25
15.	2(1H)-Pyridinone	95	C5H5NO	22
16.	3-Cyclohexene-1-carboxaldehyde, 1-methyl	124	C8H12O	22
17.	Furan, 2,5-dimethyl-	96	C6H8O	22
18.	2H-Pyran-2-one, 4,6-dimethyl-	124	C7H8O2	18
19.	2-Nonyne	124	C9H16	16
20.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	000142-83-6	575	57	32	0	95	19	37	10	39	8831
2.	*47	001530-88-7	567	34	59	3	126	40	20	0	39	9418
3.	*43	001739-84-0	564	34	51	1	99	43	18	0	39	9093
4.	*42	020521-42-0	576	50	38	1	86	27	17	2	35	7605
5.	*38	001072-68-0	569	37	62	2	107	46	14	0	41	8697
6.	*38	000694-48-4	559	62	33	2	84	48	14	8	38	9033
7.	*37	000930-62-1	565	35	57	1	81	41	13	0	35	9170
8.	35	000067-51-6	117571	49	41	0	58	52	11	8	41	9025
9.	35	000067-51-6	117570	43	48	1	62	52	11	11	41	9072
10.	32	019447-29-1	4863	51	47	2	50	48	9	16	36	6134
11.	*30	030086-02-3	4760	52	37	0	45	60	9	0	46	5223
12.	*25	002758-18-1	594	35	69	3	99	53	7	0	35	9094
13.	*25	000067-51-6	117569	33	49	1	99	52	7	4	37	8960
14.	25	000067-51-6	561	42	47	0	62	52	7	2	35	8996
15.	*22	000142-08-5	117537	34	29	1	45	62	5	11	40	5604
16.	*22	000931-96-4	4804	35	71	1	29	65	5	0	39	6652
17.	*22	000625-86-5	117584	42	56	2	89	61	5	0	39	8899
18.	*18	000675-09-2	4695	46	33	0	22	70	3	0	44	8158
19.	*16	019447-29-1	120427	45	41	1	42	59	3	16	36	6316
20.	16	002758-18-1	117591	45	46	1	42	57	3	0	35	9234

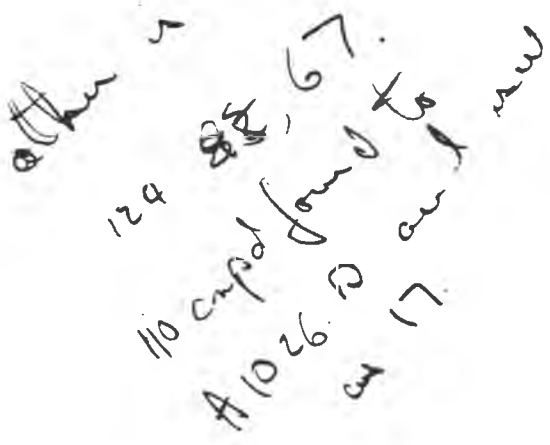
Peak 17



Scan 308 (10.160 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	222	62.00	372	82.00	4987	111.00	401
49.95	1177	62.95	701	82.95	150	118.95	158
50.95	1597	66.00	416	84.00	116	121.45	53
51.95	757	67.00	10000	84.40	70	124.05	1116
53.05	2302	67.95	1016	91.05	497	124.95	201
54.05	2731	75.05	231	91.95	371		
54.95	806	77.05	669	95.05	1772		
58.75	94	78.00	77	95.95	157		
59.25	114	79.00	235	98.00	38		
59.65	107	80.00	214	109.00	1103		
59.90	87	81.00	959	110.00	5099		



Compounds from Proctor and Gamble A0331.D

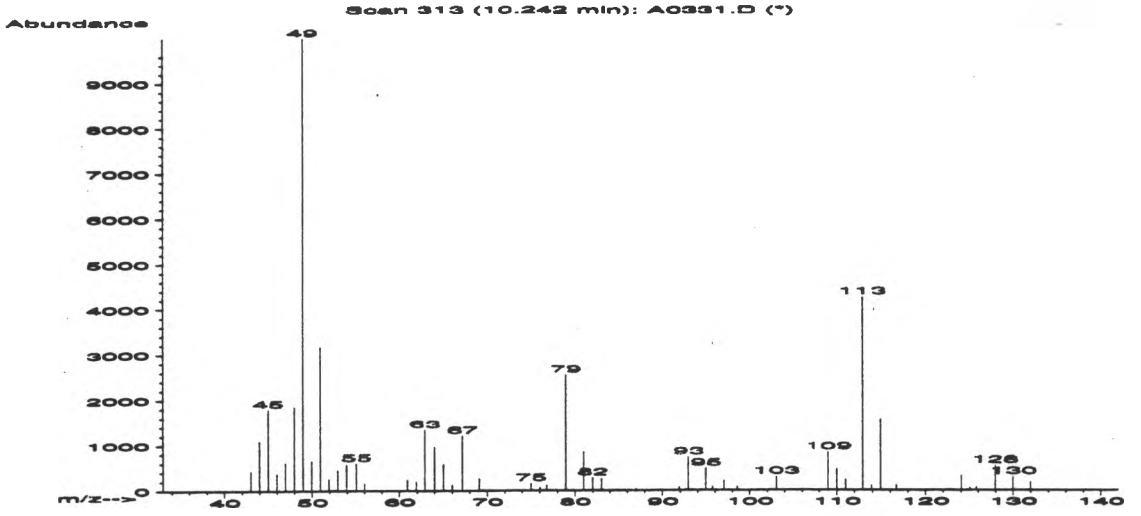
Scan 308 (10.160 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3-Octyne, 2-methyl-	124	C9H16	70
2.	2,4-Hexadiene	82	C6H10	60
3.	2,3-DIMETHYL-2-CYCLOPENTEN-1-ONE	110	C7H10O	58
4.	1,4-Hexadiene	82	C6H10	58
5.	1,3-Butadiene, 2,3-dimethyl-	82	C6H10	49
6.	2,4-Hexadiene	82	C6H10	47
7.	Bicyclo[3.1.0]hexane	82	C6H10	47
8.	1,4-Hexadiene	82	C6H10	47
9.	3-Hexyne	82	C6H10	47
10.	Cyclohexene	82	C6H10	46
11.	Cyclohexene	82	C6H10	46
12.	4-Octyne, 2-methyl-	124	C9H16	43
13.	Cyclohexene	82	C6H10	43
14.	Cyclopentane, methylene-	82	C6H10	38
15.	Cyclopropane, 1,2-dimethyl-3-methylene-	82	C6H10	38
16.	3-Hexyne	82	C6H10	35
17.	1H-Imidazole-2-carboxaldehyde, 1-methyl-	110	C5H6N2O	35
18.	1H-Imidazole-2-carboxaldehyde, 1-methyl-	110	C5H6N2O	35
19.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	18
20.	Cyclopentene, 1-methyl-	82	C6H10	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*70	055402-15-8	120437	75	22	2	80	28	41	26	66	8905
2.	*60	000592-46-1	116772	63	32	1	77	37	35	0	64	8993
3.	*58	001121-05-7	2188	55	43	1	70	29	32	0	49	9136
4.	*58	000592-45-0	116766	60	42	0	89	33	32	0	56	8980
5.	*49	000513-81-5	116776	46	55	1	84	37	23	0	44	8983
6.	*47	000592-46-1	116773	43	56	1	99	37	20	0	39	8956
7.	*47	000285-58-5	116792	34	42	1	99	39	20	7	40	8243
8.	*47	000592-45-0	116767	35	32	1	87	37	20	0	41	8980
9.	*47	000928-49-4	116764	47	39	1	81	37	20	9	38	8835
10.	*46	000110-83-8	116787	57	33	1	99	45	20	0	49	8355
11.	*46	000110-83-8	116786	53	46	1	88	45	20	0	47	8229
12.	*43	010306-94-2	120439	37	58	2	73	43	18	18	40	8411
13.	*43	000110-83-8	116788	42	48	2	98	45	18	0	39	8287
14.	*38	001528-30-9	116785	39	41	1	99	39	14	11	37	8836
15.	38	062338-02-7	116779	53	42	0	99	47	14	0	39	8437
16.	*35	000928-49-4	116763	33	72	0	56	54	11	0	41	8686
17.	*35	013750-81-7	118817	40	52	2	50	55	11	5	38	5470
18.	*35	013750-81-7	2107	45	48	2	50	55	11	7	40	5765
19.	*18	001072-91-9	2139	48	33	0	39	69	3	0	46	5035
20.	*14	000693-89-0	116781	38	48	3	177	70	2	0	39	8509

Peak 18



Scan 313 (10.242 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	426	53.95	570	75.05	159	95.70	78
43.95	1091	55.05	602	76.05	64	97.05	211
44.95	1793	56.00	151	76.80	116	98.55	78
45.95	375	60.90	235	78.95	2555	103.05	297
46.95	611	61.90	199	81.00	848	109.00	841
47.95	1846	62.90	1337	82.00	278	110.00	464
48.95	10000	64.00	962	83.00	255	111.00	227
49.95	662	65.00	586	87.00	42	112.90	4280
50.95	3168	66.00	130	91.90	70	113.90	98
51.95	249	67.15	1203	92.95	734	114.90	1571
52.95	450	69.05	262	94.95	485	116.70	108

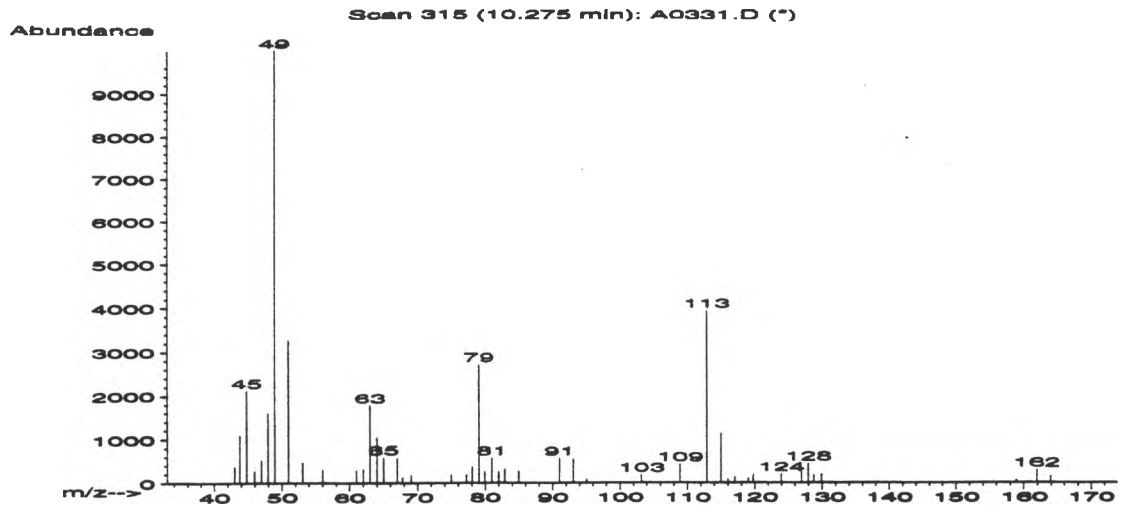
Scan 313 (10.242 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	320						
125.05	59						
125.80	61						
127.95	546						
130.00	297						
132.00	177						

Peak 18 cont'd

bis-(chloromethyl)-sulphonyl



Scan 315 (10.275 min): A0331.D

Modified:scaled clipped

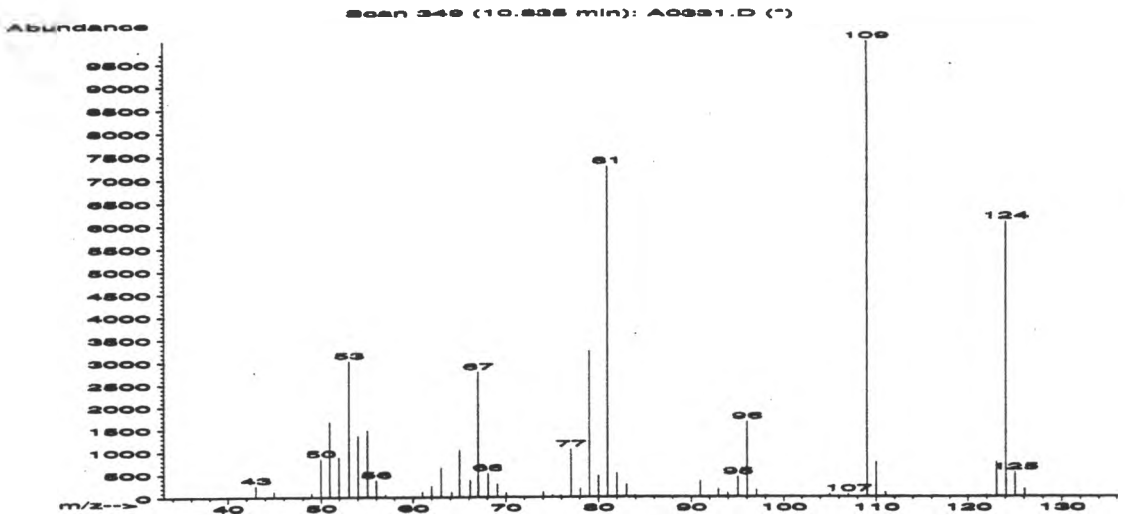
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	370	62.00	318	79.90	260	115.00	1141
43.80	1090	63.00	1781	81.00	573	116.00	79
44.80	2116	64.00	1043	82.00	250	117.05	131
45.95	273	65.00	585	82.90	321	119.05	107
46.95	530	67.00	557	85.00	272	119.80	189
47.95	1600	67.80	124	91.00	564	123.95	201
48.95	10000	69.05	182	93.05	545	126.95	256
50.95	3262	74.95	190	95.05	80	127.95	447
53.05	469	77.20	190	103.20	184	128.75	176
56.00	300	78.05	373	108.90	433	129.90	193
61.00	288	79.05	2723	112.90	3947	158.90	75

Scan 315 (10.275 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
161.90	297						
163.90	149						

Peak 19



Scan 349 (10.835 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	248	59.00	33	70.80	26	83.90	27
44.95	122	61.00	114	74.05	106	91.00	352
48.95	80	62.00	241	75.05	46	91.95	19
49.95	841	63.00	645	75.95	42	92.95	173
50.95	1672	64.15	106	77.05	1056	93.95	87
51.95	877	65.00	1035	78.05	188	95.05	439
53.05	3023	66.15	380	79.05	3244	96.05	1674
54.05	1353	67.00	2773	80.00	463	97.05	154
55.05	1475	68.05	528	81.00	7233	98.05	24
56.00	367	69.05	283	82.00	516	105.00	57
57.00	56	70.05	93	83.00	272	105.90	11

Scan 349 (10.835 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	61						
109.00	10000						
110.00	762						
111.00	103						
119.95	26						
121.95	36						
123.05	765						
124.05	6049						
125.05	533						
126.05	170						

Compounds from Proctor and Gamble A0331.D

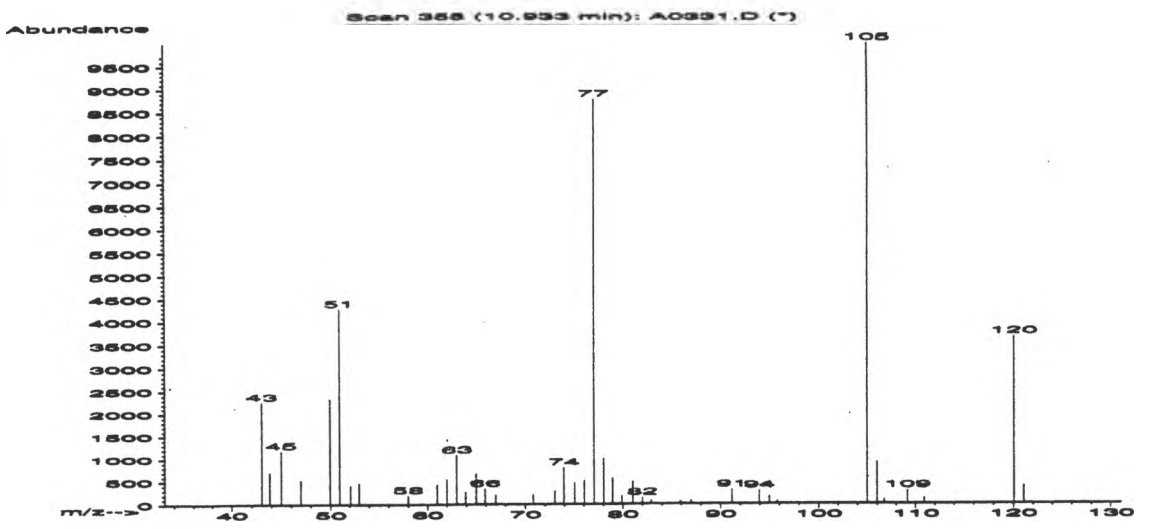
Scan 349 (10.835 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-methoxy-	124	C7H8O2	76
2.	Cycloopent-2-ene-1-one, 2,3,4-trimethyl-	124	C8H12O	76
3.	2-Cyclopenten-1-one, 3,4,5-trimethyl-	124	C8H12O	74
4.	Phenol, 4-methoxy-	124	C7H8O2	68
5.	2-Cyclopenten-1-one, 3,4,4-trimethyl-	124	C8H12O	64
6.	Phenol, 2-methoxy-	124	C7H8O2	64
7.	Phenol, 2-methoxy-	124	C7H8O2	62
8.	Phenol, 2-methoxy-	124	C7H8O2	62
9.	2-Acetyl-5-methylfuran	124	C7H8O2	58
10.	Phenol, 2-methoxy-	124	C7H8O2	58
11.	2-Cyclopenten-1-one, 2,3,4-trimethyl-	124	C8H12O	58
12.	Pyridine, 3-methyl-, 1-oxide	109	C6H7NO	43
13.	1-METHYL-2-PYRROLECARBOXALDEHYDE	109	C6H7NO	38
14.	3-Pyridinol, 6-methyl-	109	C6H7NO	38
15.	2(1H)-Pyridinone, 1-methyl-	109	C6H7NO	30
16.	Pyridine, 2-methyl-, 1-oxide	109	C6H7NO	27
17.	4,5-DIMETHYL-2-PYRIMIDONE	124	C6H8N2O	25
18.	1,3-PENTADIENE, 2,3-DIMETHYL-	96	C7H12	20
19.	QUINUCLIDINEBORANE	125	C7H16BN	14
20.	1,4-Hexadiene, 5-methyl-	96	C7H12	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*76	000090-05-1	120382	80	18	1	87	25	45	29	64	9170
2.	*76	083321-16-8	4858	75	27	0	70	21	45	35	74	9403
3.	*74	055683-21-1	120406	65	33	1	82	17	44	12	53	8970
4.	*68	000150-76-5	120386	71	21	1	79	25	40	18	58	9177
5.	*64	030434-65-2	4785	55	39	1	92	22	37	14	49	9228
6.	*64	000090-05-1	120383	63	28	1	80	33	37	0	64	9292
7.	*62	000090-05-1	120380	77	31	2	77	28	36	19	50	9044
8.	*62	000090-05-1	120377	74	24	2	92	26	36	27	60	9066
9.	*58	001193-79-9	4688	52	34	1	99	28	32	0	46	9212
10.	*58	000090-05-1	120379	62	27	2	99	30	32	29	49	9164
11.	*58	028790-86-5	4783	62	38	0	63	35	32	0	56	9548
12.	*43	001003-73-2	118784	56	29	2	83	50	18	14	49	8256
13.	*38	001192-58-1	2034	37	65	3	78	48	14	0	41	8135
14.	*38	001121-78-4	2050	36	59	3	84	53	14	4	43	8063
15.	*30	000694-85-9	2043	35	42	2	99	57	9	10	43	7976
16.	*27	000931-19-1	2040	49	31	1	77	57	8	4	43	7872
17.	*25	034939-17-8	4681	52	37	1	49	64	7	0	44	6654
18.	*20	000000-00-0	626	72	22	0	72	70	4	31	58	3866
19.	*14	000000-00-0	5024	45	63	2	56	69	2	0	40	4811
20.	*14	000763-88-2	619	59	32	0	72	70	2	14	41	3736

Peak 20



Scan 355 (10.933 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2250	63.00	1078	78.05	990	95.80	60
43.80	699	63.90	259	78.95	562	105.00	10000
44.95	1175	65.00	665	79.90	176	106.00	904
46.95	529	65.90	331	81.00	490	106.75	92
49.95	2317	67.00	206	82.00	146	109.15	292
50.95	4256	70.80	206	82.90	79	110.90	124
52.05	407	73.05	280	85.90	49	120.05	3636
52.95	460	73.95	797	87.00	80	121.05	385
58.00	193	75.05	458	91.15	312		
61.00	425	76.05	525	93.95	293		
62.00	549	77.05	8727	94.95	166		

Compounds from Proctor and Gamble A0331.D

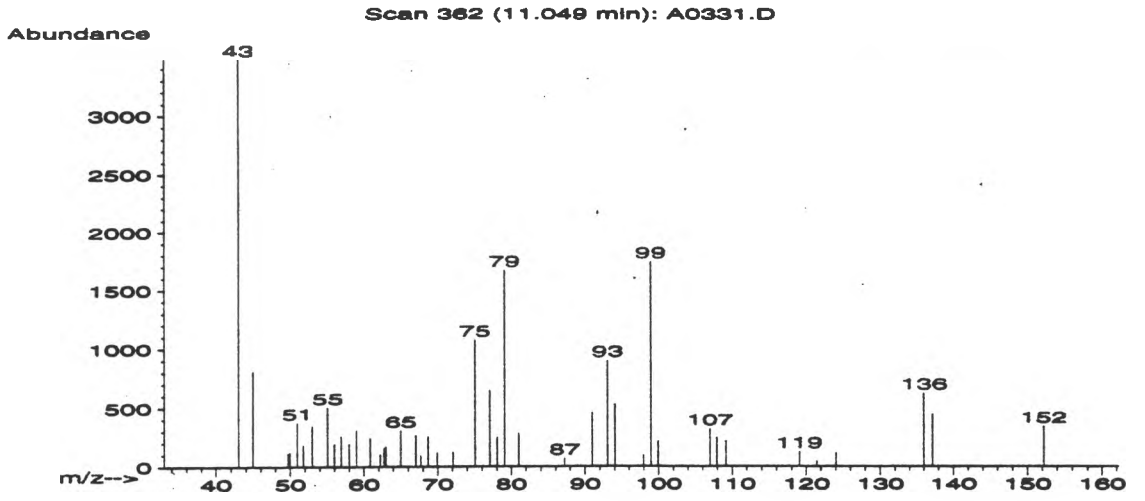
Scan 355 (10.933 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-phenyl-	120	C8H8O	94
2.	Ethanone, 1-phenyl-	120	C8H8O	94
3.	Ethanone, 1-phenyl-	120	C8H8O	91
4.	Ethanone, 1-phenyl-	120	C8H8O	91
5.	Ethanone, 1-phenyl-	120	C8H8O	91
6.	Ethanone, 1-phenyl-	120	C8H8O	91
7.	Ethanone, 1-phenyl-	120	C8H8O	90
8.	Ethanone, 1-phenyl-	120	C8H8O	87
9.	Ethanone, 1-phenyl-	120	C8H8O	87
10.	1,2-Propanedione, 1-phenyl-	148	C9H8O2	80
11.	Benzeneacetic acid, .alpha.-oxo-, methyl	164	C9H8O3	72
12.	Benzoic acid, phenyl ester	198	C13H10O2	64
13.	1,1-DIBROMO-ACETOPHENONEPHOSPHINE	276	C8H6Br2O	64
14.	2-Phenyl-3-oxetanone	148	C9H8O2	64
15.	Benzoyl chloride	140	C7H5ClO	64
16.	Benzoyl bromide	184	C7H5BrO	53
17.	Ethanone, 1-phenyl-	120	C8H8O	53
18.	2,4-Heptadien-6-ynal, (E,E)-	106	C7H6O	38
19.	Benzene, 1,3,5-trimethyl-	120	C9H12	27
20.	Benzene, (1-methylethyl)-	120	C9H12	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000098-86-2	119991	82	9	0	99	2	70	0	93	9981
2.	*94	000098-86-2	119989	82	16	0	82	2	70	0	93	9966
3.	*91	000098-86-2	119986	80	16	0	96	2	62	39	81	9821
4.	*91	000098-86-2	119993	70	19	0	94	2	62	26	70	9846
5.	*91	000098-86-2	119994	67	4	0	98	4	62	0	64	9971
6.	*91	000098-86-2	119988	75	21	0	99	2	62	0	81	9986
7.	*90	000098-86-2	119987	67	25	0	94	2	57	12	47	9899
8.	*87	000098-86-2	119985	59	33	0	99	6	54	0	56	9943
9.	*87	000098-86-2	4126	58	33	0	99	6	54	0	56	9913
10.	80	000579-07-7	11943	66	21	0	89	13	48	4	43	9615
11.	72	015206-55-0	125272	58	29	0	95	13	42	0	43	9663
12.	64	000093-99-2	128222	55	46	1	86	18	37	10	39	9203
13.	64	000000-00-0	65437	76	45	0	83	16	37	5	42	8798
14.	64	087385-78-2	11961	57	30	0	86	18	37	0	39	9655
15.	64	000098-88-4	122403	58	36	1	89	16	37	0	43	9600
16.	53	000618-32-6	27174	43	56	0	72	30	28	19	41	9340
17.	*53	000098-86-2	119992	43	37	1	99	29	28	0	40	9474
18.	38	007200-04-6	1773	51	46	3	94	50	14	12	41	7976
19.	*27	000108-67-8	120037	33	69	2	81	60	8	11	40	7980
20.	*27	000098-82-8	120011	37	52	1	99	59	8	0	39	8265

Peak 21



Scan 362 (11.049 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3480	59.00	305	75.05	1070	99.95	212
44.95	809	60.90	239	77.05	644	107.00	319
49.70	114	62.25	102	78.05	247	107.90	245
49.95	125	62.75	158	79.05	1664	109.15	216
50.95	373	63.00	167	81.00	284	119.05	123
51.80	182	65.00	301	87.25	69	121.45	45
52.95	346	67.00	265	91.00	458	124.05	114
55.05	503	67.70	94	93.05	895	136.00	624
56.00	191	68.70	252	94.05	528	137.15	444
56.90	256	69.95	116	97.95	96	152.20	340
58.00	193	72.05	122	98.95	1736		

Compounds from Proctor and Gamble A0331.D

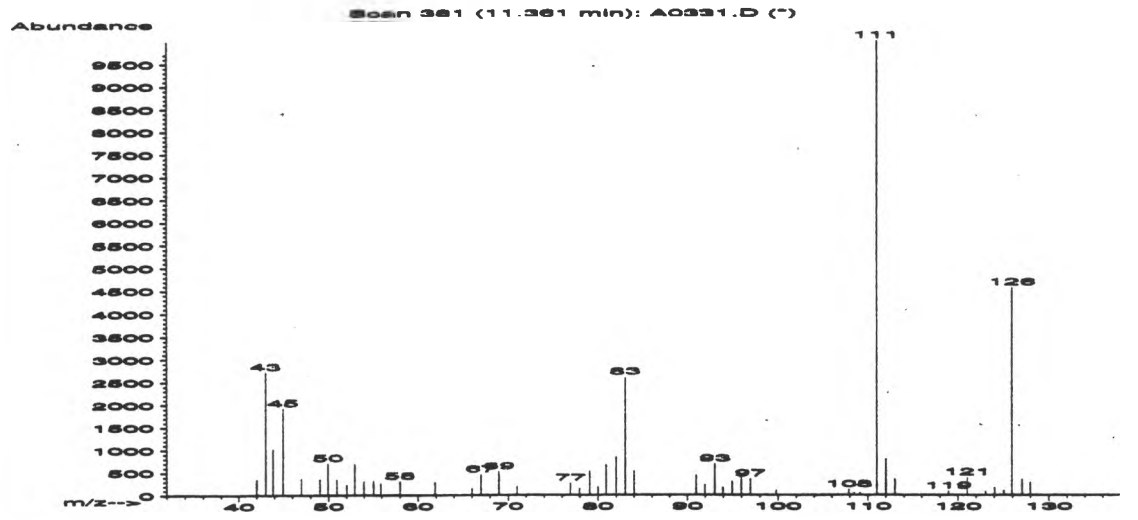
Scan 362 (11.049 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Limonene oxide	152	C10H16O	10
2.	Cyclohexanol, 1-methyl-4-(1-methyletheny	154	C10H18O	9
3.	Cyclohexanol, 2-methyl-3-(1-methyletheny	196	C12H20O2	9
4.	3,7-Decadiene-5,6-diol, 4,7-dimethyl-	198	C12H22O2	9
5.	3-METHYLISOXAZOL-5-ONE	99	C4H5NO2	9
6.	1-METHYL-3-THIAHEXYLMERCAPTAN	136	C5H12S2	9
7.	Carveol, dihydro-, cis-	154	C10H18O	8
8.	4-Terpinenyl ester of n-butanoic acid	224	C14H24O2	8
9.	cis-7-Methylenebicyclo[3.3.0]octan-2-one	136	C9H12O	8
10.	2-HYDROXY-3-CHLORO-METHYLPROPIONATE	138	C4H7ClO3	8
11.	Cyclohexanol, 2-methylene-3-(1-methyleth	196	C12H20O2	7
12.	3,5-Nonadien-7-yn-2-ol, (E,E)-	136	C9H12O	7
13.	Dihydrocarvyl acetate	196	C12H20O2	7
14.	3-Octanone, 2-methyl-	142	C9H18O	7
15.	CYCLOBUTENE-3,4-DIOL, TETRAMETHYL-	142	C8H14O2	7
16.	.beta.-Myrcene	136	C10H16	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.*	10	001195-92-2	13724	28	89	2	65	63	1	0	23	6203
2.	9	000138-87-4	124296	40	56	0	32	71	1	0	33	5256
3.	9	054845-29-3	32968	40	76	0	71	77	1	0	33	4021
4.	9	022427-95-8	33933	40	62	2	68	77	1	0	33	5835
5.*	9	001517-96-0	961	29	68	0	87	73	1	0	33	6116
6.*	9	000000-00-0	7723	30	69	0	36	72	1	0	33	4824
7.	8	038049-26-2	14709	33	61	0	23	68	1	6	26	6199
8.	8	002153-28-8	45918	40	83	1	40	68	1	0	29	5687
9.	8	084642-40-0	8003	41	59	2	97	69	1	0	28	6289
10.	8	000000-00-0	8363	33	58	1	67	68	1	0	21	6013
11.	7	054845-30-6	32974	51	69	1	74	71	1	0	27	5446
12.*	7	043142-43-4	7879	28	72	2	87	77	1	0	26	5196
13.	7	020777-49-5	32973	33	94	3	99	78	1	0	22	6055
14.	7	000923-28-4	10171	37	51	0	99	78	1	0	25	5642
15.	7	000000-00-0	10040	39	43	1	99	76	1	0	29	6137
16.*	7	000123-35-3	121969	31	76	3	101	78	1	0	27	4417

Peak 22



Scan 381 (11.361 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	344	55.05	310	80.00	177	96.95	357
43.00	2714	55.90	257	80.90	666	99.80	102
43.80	1010	58.00	306	82.00	847	107.90	123
44.95	1915	61.90	288	83.00	2601	108.50	42
46.95	364	66.00	144	84.00	527	109.15	52
49.05	350	67.00	458	91.00	439	111.00	10000
49.95	703	68.95	519	91.95	228	112.00	798
50.95	339	70.95	194	93.05	689	113.00	350
52.05	230	76.95	261	93.95	163	118.95	88
52.95	689	77.95	148	94.95	299	121.05	390
53.95	297	79.05	526	95.95	439	123.05	78

Scan 381 (11.361 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.05	161						
125.05	97						
125.95	4560						
127.05	348						
127.95	275						

Compounds from Proctor and Gamble A0331.D

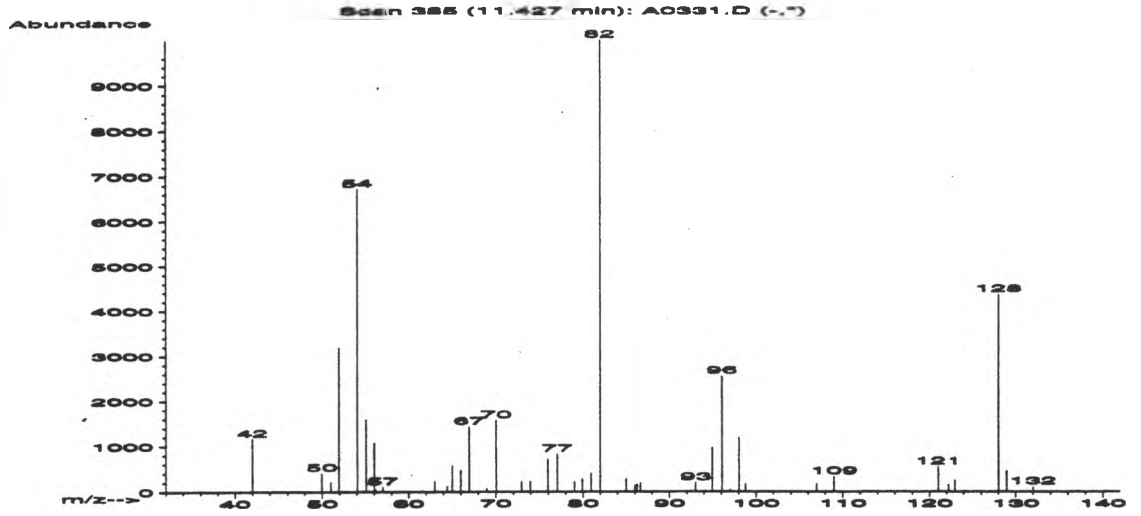
Scan 381 (11.361 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	86
2.	Ethanone, 1-(3-thienyl)-	126	C6H6OS	86
3.	Ethanone, 1-(3-thienyl)-	126	C6H6OS	80
4.	3,4,4-Trimethyl-2-pentenal	126	C8H14O	78
5.	3-Octen-2-one, (E)-	126	C8H14O	78
6.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	72
7.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	72
8.	1H-Pyrazole, 3-ethyl-4,5-dihydro-1,4-dim	126	C7H14N2	64
9.	Thiophene, 2-(1-methylethyl)-	126	C7H10S	59
10.	2-ETHYL-5-METHYLTHIOPHENE	126	C7H10S	50
11.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	45
12.	1,1,3-TRIMETHYL-1-SILACYCLO-3-PENTENE	126	C7H14Si	42
13.	Crotonaldehyde, isopropylhydrazone	126	C7H14N2	40
14.	Ethanone, 1-(3-hydroxy-2-furanyl)-	126	C6H6O3	38
15.	2(3H)-Furanone, 5-ethenyldihydro-5-methy	126	C7H10O2	38
16.	2(3H)-Furanone, 5-ethenyldihydro-5-methy	126	C7H10O2	38
17.	2-Cyclopenten-1-one, 3-methoxy-4-methyl-	126	C7H10O2	38
18.	4(1H)-Pyrimidinone, 2-amino-	111	C4H5N3O	38
19.	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	37
20.	Benzenamine, 3-fluoro-	111	C6H6FN	37

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	000088-15-3	120500	66	30	0	80	10	53	3	47	9892
2.	*86	001468-83-3	120504	62	32	0	83	6	53	5	49	9898
3.	*80	001468-83-3	5115	44	43	1	99	14	48	0	44	9864
4.	*78	065275-95-8	5293	30	7	0	88	7	46	9	42	9571
5.	*78	018402-82-9	120575	36	15	0	83	7	46	5	38	9546
6.	*72	000088-15-3	120501	48	53	1	83	17	42	0	44	9721
7.	*72	000088-15-3	5114	43	44	0	85	18	42	0	44	9913
8.	*64	075011-91-5	5272	50	54	2	77	21	37	0	44	9822
9.	*59	004095-22-1	5250	44	42	3	82	22	33	13	38	9635
10.	*50	000000-00-0	5251	45	43	3	89	31	25	0	40	9560
11.	*45	000088-15-3	120502	39	50	1	93	23	19	1	36	9836
12.	*42	003528-14-1	5282	36	69	3	99	26	17	0	35	9775
13.	*40	018631-71-5	5257	35	76	2	76	34	16	0	35	9559
14.	*38	003420-59-5	5122	45	43	1	61	51	14	0	44	9567
15.	38	001073-11-6	120556	38	71	2	99	36	14	0	33	9353
16.	38	001073-11-6	5200	38	71	2	99	36	14	0	33	9326
17.	*38	007180-61-2	5206	35	54	1	57	52	14	14	43	9392
18.	*38	000108-53-2	2308	36	44	2	99	50	14	17	40	8951
19.	37	003073-66-3	5465	38	60	0	86	43	13	0	33	9090
20.	*37	000372-19-0	2338	38	59	1	77	44	13	0	33	8997

Peak 23



Scan 385 (11.427 min): A0331.D

Modified:subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	1154	66.00	475	82.00	10000	107.00	166
49.95	409	67.00	1433	85.00	293	109.00	331
51.00	212	68.95	68	86.00	133	121.05	544
51.95	3189	70.05	1568	86.25	164	122.20	148
54.05	6717	72.95	218	86.65	193	122.95	250
55.05	1584	73.95	229	93.00	202	124.05	14
56.00	1076	75.95	720	94.95	965	128.05	4357
56.95	104	77.05	828	96.05	2549	129.00	455
63.00	232	79.00	223	97.05	49	132.00	104
64.40	119	79.95	277	98.05	1183		
65.00	569	80.95	403	98.80	162		

Scan 385 (11.427 min): A0331.D

Compounds from Proctor and Gamble A0331.D

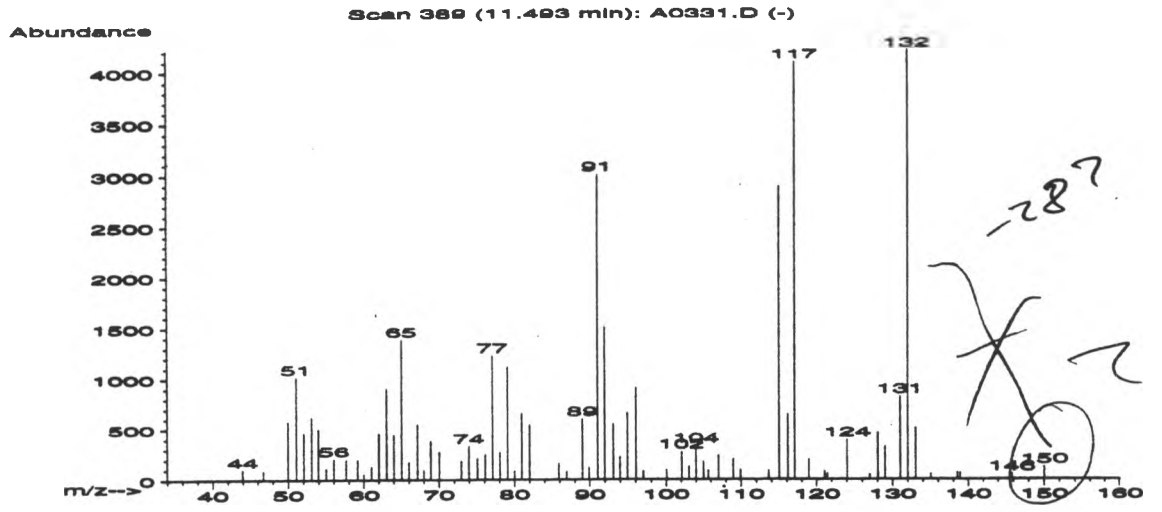
Scan 385 (11.427 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Nitrobenzene-d5	123	C6D5NO2	49
2.	1H-Pyrazole-4-carboxylic acid, 3-methyl-	126	C5H6N2O2	40
3.	1,3-Isobenzofurandione, hexahydro-	154	C8H10O3	33
4.	1H-Imidazole, 4-methyl-	82	C4H6N2	17
5.	Isoxazole, 3,5-dimethyl-	97	C5H7NO	17
6.	2-Pentenoic acid, 3-methyl-, methyl este	128	C7H12O2	10
7.	3-Pentenoic acid, 3-methyl-, methyl este	128	C7H12O2	9
8.	2-Hexyne	82	C6H10	8
9.	BICYCLO(3.2.1)OCTAN-2-ONE-EXO-6-EXO-7-D2	124	C8H10D2O	7
10.	Ethanamine, N-cyclopentylidene-	111	C7H13N	7
11.	1-OCTEN-3-YL BUTYRATE	198	C12H22O2	7
12.	1,2-Nonadiene	124	C9H16	7
13.	1,2-Nonadiene	124	C9H16	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	000000-00-0	4529	51	44	0	80	36	23	0	44	9661
2.	40	040704-11-8	5093	38	72	2	85	32	16	2	31	9179
3.	33	000085-42-7	124143	37	56	2	79	32	10	0	21	9164
4.	*17	000822-36-6	116748	28	68	1	96	55	3	0	29	9050
5.	17	000300-87-8	117634	33	68	1	72	54	3	0	21	8930
6.	*10	050652-79-4	5791	37	74	1	57	72	1	0	39	3844
7.	* 9	041654-12-0	5795	30	51	0	65	77	1	0	33	3733
8.	* 8	000764-35-2	116760	23	66	1	99	67	1	0	29	8838
9.	7	019329-35-2	4836	36	66	1	79	71	1	0	21	7808
10.	7	054966-05-1	2368	38	67	1	54	72	1	0	28	8358
11.	7	000000-00-0	33908	38	92	1	55	79	1	0	28	6513
12.	7	022433-33-6	120434	39	50	2	53	79	1	0	29	5923
13.	7	022433-33-6	4866	35	59	1	52	79	1	0	22	5960

Peak 24



Scan 389 (11.493 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	98	60.00	52	72.95	184	86.90	80
46.70	85	61.00	129	73.95	330	89.00	601
49.95	575	62.00	457	75.05	207	89.90	121
51.05	1017	63.00	898	76.05	244	91.00	2995
52.05	461	64.00	442	77.05	1224	91.95	1503
53.05	619	65.00	1382	78.05	269	93.05	550
53.95	497	66.00	170	79.05	1112	93.95	221
55.00	111	67.15	545	80.00	85	94.95	657
56.00	205	68.00	96	81.00	650	96.05	904
57.65	196	68.90	384	82.00	542	97.00	86
59.15	193	70.05	277	85.90	158	100.05	94

Scan 389 (11.493 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.05	273	117.05	4096	135.00	52		
103.05	128	118.95	192	138.50	66		
104.00	332	121.05	80	138.90	63		
105.00	174	121.45	56	145.80	50		
105.65	87	124.05	390	150.05	119		
107.00	235	127.00	47				
109.00	195	128.05	455				
109.90	97	129.00	322				
113.65	88	131.00	817				
115.00	2883	132.00	4217				
116.15	643	133.00	504				

Compounds from Proctor and Gamble A0331.D

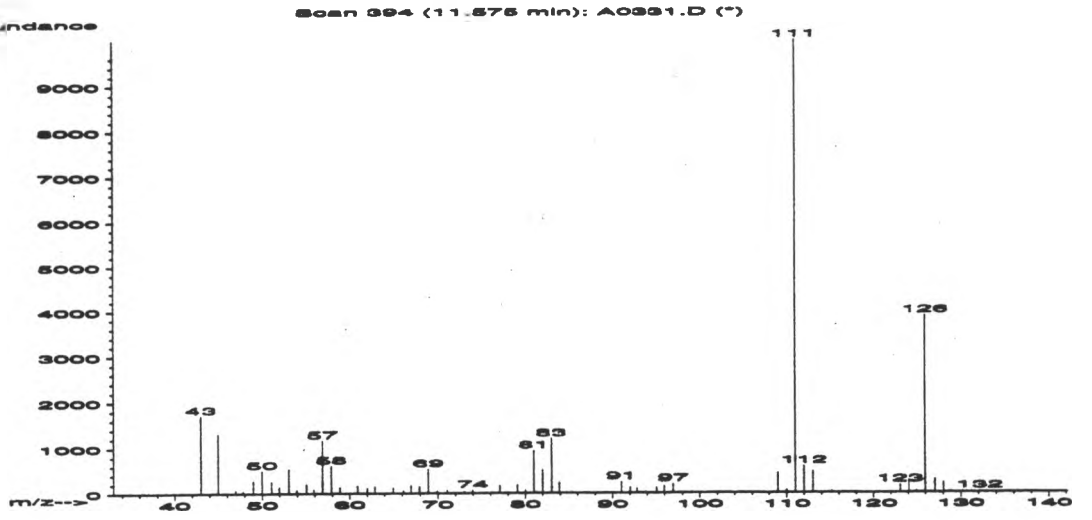
Scan 389 (11.493 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1-methyl-4-(1-methylethenyl)-	132	C10H12	92
2.	Benzene, methyl(1-methylethenyl)-	132	C10H12	81
3.	BENZENE, 1-ISOPROPENYL-?-METHYL-	132	C10H12	76
4.	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	70
5.	Benzene, (2-methyl-1-propenyl)-	132	C10H12	64
6.	Benzene, ethenyl-, dimethyl deriv.	132	C10H12	64
7.	Benzene, 4-ethenyl-1,2-dimethyl-	132	C10H12	64
8.	Benzene, (1-methylenepropyl)-	132	C10H12	64
9.	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	58
10.	Benzene, 2-butenyl-	132	C10H12	58
11.	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	53
12.	Benzene, (2-methyl-1-propenyl)-	132	C10H12	53
13.	Benzene, (2-methyl-2-propenyl)-	132	C10H12	49
14.	Benzene, 1-methyl-4-(1-methylethenyl)-	132	C10H12	49
15.	cis-3-(1-Butynyl)-4-vinylcyclopentene	146	C11H14	43
16.	Benzene, (1-methyl-1-propenyl)-, (Z)-	132	C10H12	42
17.	1R-METHYL-2T-PHENYLCYCLOPROPANE	132	C10H12	41
18.	Benzene, 1-methyl-4-(1-methylethenyl)-	132	C10H12	38
19.	1H-Benzimidazole, 2-methyl-	132	C8H8N2	35
20.	Benzene, (2-methyl-1-propenyl)-	132	C10H12	30

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*92	001195-32-0	121408	81	40	0	93	28	64	0	93	9689
2.	*81	026444-18-8	121411	63	41	1	99	18	49	0	64	9601
3.	*76	026444-18-8	7009	78	33	1	96	22	45	28	74	9662
4.	*70	001587-04-8	121407	73	43	1	97	27	41	0	81	9688
5.	*64	000768-49-0	121402	66	48	2	90	24	37	6	45	9510
6.	*64	027576-03-0	7016	66	48	2	90	24	37	6	45	9510
7.	*64	027831-13-6	7014	53	48	1	71	25	37	0	49	9314
8.	*64	002039-93-2	6998	69	47	1	93	34	37	0	76	9323
9.	*58	002039-89-6	7012	70	45	2	95	34	32	20	59	9466
10.	*58	001560-06-1	121398	66	39	0	80	35	32	6	53	9066
11.	*53	005379-20-4	7015	58	45	2	99	39	28	0	56	9228
12.	*53	000768-49-0	6996	59	50	2	97	40	28	5	55	9312
13.	*49	003290-53-7	6997	59	46	1	97	39	23	6	45	9048
14.	*49	001195-32-0	121410	54	53	1	75	40	23	6	47	8809
15.	*43	092901-56-9	11486	36	31	0	87	50	18	2	43	7386
16.	*42	000767-99-7	6994	63	52	3	135	60	17	0	64	9103
17.	*41	005070-01-9	7019	58	47.	2	148	54	16	0	51	8809
18.	*38	001195-32-0	7008	49	50	1	99	54	14	0	46	7804
19.	*35	000615-15-6	121380	43	80	3	99	54	11	8	43	5986
20.	*30	000768-49-0	121403	62	46	2	143	59	9	0	46	9337

BKME Peak 25



Scan 394 (11.575 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1707	55.90	89	68.95	532	83.90	226
44.95	1314	56.90	1162	69.95	53	91.00	250
46.95	74	57.90	604	71.05	69	92.05	120
47.80	46	58.90	137	72.95	38	92.80	100
48.95	282	60.90	165	73.95	69	93.80	30
49.95	501	62.00	117	77.05	174	95.05	116
51.05	261	62.90	159	79.05	188	95.95	151
51.95	152	65.00	121	80.00	65	96.95	202
53.05	538	66.15	60	81.00	931	99.05	26
53.95	77	67.00	177	82.00	505	106.90	15
55.05	203	67.95	147	83.00	1200	109.00	436

Scan 394 (11.575 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.00	65	132.15	27				
111.00	10000						
112.00	591						
113.00	470						
115.15	38						
123.05	180						
124.05	281						
124.95	44						
125.95	3892						
127.05	289						
128.05	223						

Compounds from Proctor and Gamble A0331.D

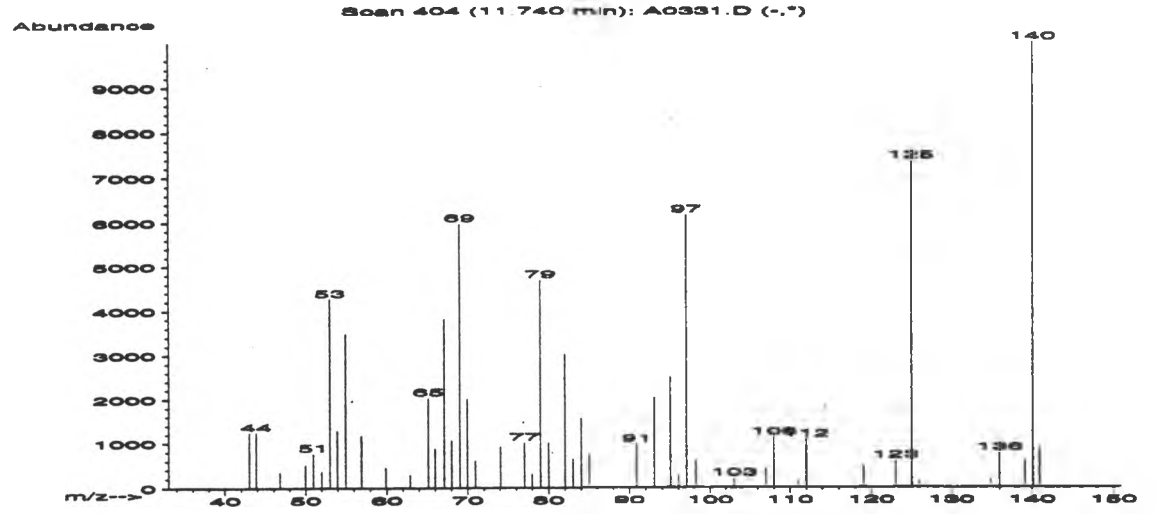
Scan 394 (11.575 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(3-thienyl)-	126	C6H6OS	87
2.	3-Octen-2-one, (E)-	126	C8H14O	78
3.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	72
4.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	72
5.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	72
6.	Thiophene, 2-(1-methylethyl)-	126	C7H10S	64
7.	2-ETHYL-5-METHYLTHIOPHENE	126	C7H10S	53
8.	Ethanone, 1-(3-thienyl)-	126	C6H6OS	53
9.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	43
10.	3-Thiophenecarboxylic acid	128	C5H4O2S	38
11.	Cyclohexane, 1,2,4-trimethyl-, (1.alpha.	126	C9H18	38
12.	3-Buten-2-one, 3-methyl-, dimethylhydraz	126	C7H14N2	36
13.	3,4-Dihydro-4,4,6-trimethyl-2H-pyran	126	C8H14O	36
14.	3-METHYL-(2,6-DIMETHYLHEPTYL)-2-PENTEN-5	238	C15H26O2	36
15.	Ethanone, 1-(2-thienyl)-	126	C6H6OS	35
16.	2-Thiophenecarboxaldehyde	112	C5H4OS	33
17.	2-Aminopyrimidin-1-oxide	111	C4H5N3O	32
18.	2-ISOPROPENYL-2-OXAZOLINE	111	C6H9NO	32
19.	2-Thiophenecarboxaldehyde	112	C5H4OS	28
20.	THIOPHENE-2-CARBOXAMIDE	127	C5H5NOS	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	001468-83-3	5115	74	15	1	89	13	54	20	76	9919
2.	*78	018402-82-9	120575	35	14	0	70	7	46	5	38	9821
3.	*72	000088-15-3	120501	54	47	3	84	19	42	0	47	9867
4.	*72	000088-15-3	120500	64	30	1	72	19	42	0	50	9838
5.	*72	000088-15-3	120502	55	33	2	74	20	42	0	49	9874
6.	*64	004095-22-1	5250	62	25	2	74	23	37	17	47	9800
7.	*53	000000-00-0	5251	45	43	2	70	26	28	0	40	9823
8.	*53	001468-83-3	120504	43	43	1	83	26	28	0	39	9844
9.	*43	000088-15-3	5114	37	50	0	51	44	18	0	41	9795
10.	38	000088-13-1	5681	46	36	1	72	36	14	2	37	9303
11.	*38	007667-60-9	5470	29	84	3	99	23	14	0	27	9829
12.	*36	075268-10-9	5256	30	73	3	91	27	12	0	26	9821
13.	*36	000000-00-0	5358	30	28	1	69	26	12	0	27	9828
14.	36	053042-71-0	51785	39	47	2	70	27	12	0	29	9315
15.	*35	000088-15-3	120503	36	46	0	32	51	11	0	41	9346
16.	33	000098-03-3	118960	40	57	2	92	35	10	0	29	7500
17.	*32	035034-15-2	2307	29	58	2	71	48	9	0	33	9170
18.	*32	000000-00-0	2344	28	53	3	81	50	9	0	33	8628
19.	28	000098-03-3	2418	42	55	2	90	38	8	0	29	7261
20.	*27	005813-89-8	5507	48	31	0	58	60	8	8	41	9280

Peak 26



Scan 404 (11.740 min): A0331.D

Modified:subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1239	62.90	297	79.05	4677	98.20	599
43.85	1244	65.15	2019	80.00	1007	103.05	204
46.80	343	66.00	877	82.00	3026	107.00	418
49.95	510	67.10	3805	83.00	650	108.00	1118
50.95	761	68.05	1058	84.00	1564	111.00	130
52.00	367	69.05	5944	85.00	742	112.00	1072
53.05	4251	69.95	2009	90.90	970	119.05	478
53.95	1281	70.95	613	93.05	2028	123.05	594
55.00	3476	74.05	919	95.05	2497	125.05	7341
56.90	1174	77.05	1007	96.05	265	126.00	153
59.90	450	78.00	306	97.05	6144	134.90	181

Scan 404 (11.740 min): A0331.D

Modified:subtracted scaled

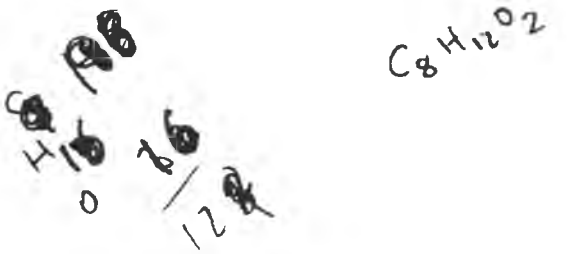
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
136.00	761						
139.15	599						
140.15	10000						
140.95	882						

Scan 404 (11.740 min): A0331.D

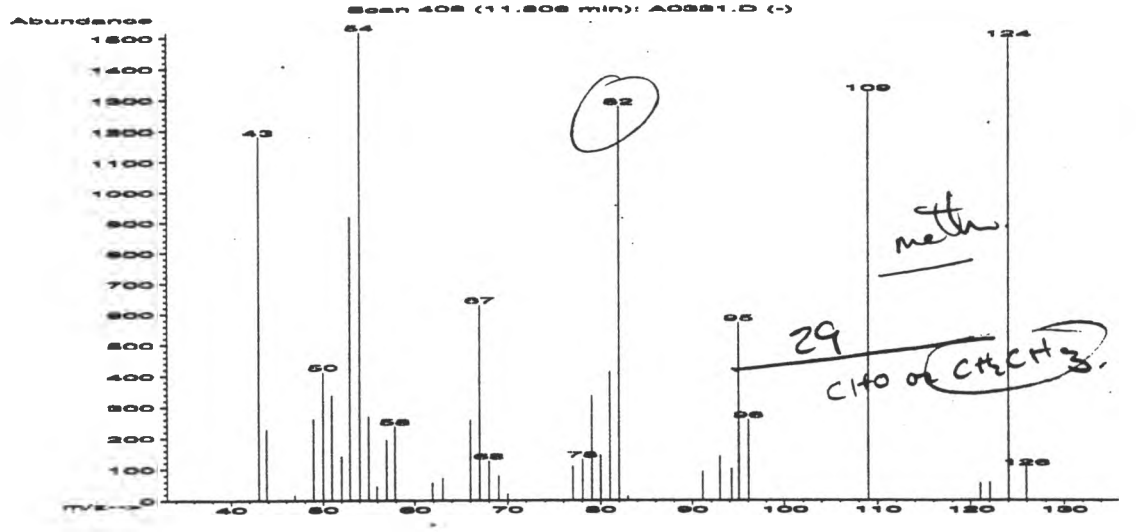
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-METHYL-3-OXIME-1-CYCLOHEXEN-3-ONE	125	C7H11NO	62
2.	1,4-Benzenediol, 2-methoxy-	140	C7H8O3	27
3.	2-Azabicyclo[2.2.2]octan-3-one	125	C7H11NO	25
4.	Methyl cyclopentylidenacetate	140	C8H12O2	25
5.	3-Octyne	110	C8H14	17
6.	2,3-Hexadiene, 2-methyl-	96	C7H12	17
7.	1,2-Benzenediol, 3-methoxy-	140	C7H8O3	16
8.	3-Methoxy-pyrocatechol	140	C7H8O3	16
9.	1,3-Cyclopentanedione, 2-acetyl-	140	C7H8O3	14
10.	Z-Citral	152	C10H16O	12
11.	ISONICOTINIC ACID-.BETA.-D2	123	C6H3D2NO2	10
12.	Uracil, 5-ethyl-	140	C6H8N2O2	10
13.	2,5-Dimethoxypyrimidine	140	C6H8N2O2	10
14.	Spiro[4.5]dec-6-ene	136	C10H16	9
15.	3H-Pyrazol-3-one, 2,4-dihydro-2,4,4,5-te	140	C7H12N2O	9
16.	Thiophene, 3-(1,1-dimethylethyl)-	140	C8H12S	9
17.	Benzenethiol, 2-amino-	125	C6H7NS	9
18.	cis-2-Oxabicyclo(4.4.0)decane	140	C9H16O	9
19.	Methyl-(endo-tricyclo[2.2.0.0(2,6)]hex-3	110	C7H10O	9
20.	4H-Pyran-4-one, 2-methoxy-6-methyl-	140	C7H8O3	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*62	000000-00-0	5006	59	63	1	73	30	36	0	56	7128
2.	*27	000824-46-4	9120	44	47	1	97	58	8	0	39	8826
3.	*25	003306-69-2	5019	42	36	2	73	52	7	11	37	6267
4.	25	000000-00-0	9205	34	68	0	54	42	7	0	25	8043
5.	17	015232-76-5	2218	39	74	1	68	54	3	0	29	4407
6.	17	029212-09-7	622	37	77	0	58	55	3	0	25	4748
7.	*16	000934-00-9	9119	35	66	2	83	57	3	2	37	8787
8.	*16	000000-00-0	9121	35	66	2	83	57	3	2	37	8787
9.	*14	003859-39-0	9106	37	62	3	96	66	2	0	39	8061
10.	12	000106-26-3	123954	39	57	3	242	56	2	0	29	3856
11.	*10	055090-51-2	4523	43	65	3	60	78	1	12	38	5249
12.	*10	004212-49-1	9060	49	42	1	85	67	1	11	31	7773
13.	*10	016290-94-1	9056	33	80	2	84	76	1	0	39	7700
14.	9	000697-28-9	8145	50	46	0	34	80	1	5	36	4135
15.	* 9	003201-25-0	9129	42	46	1	90	71	1	7	30	8069
16.	* 9	001689-79-8	122459	36	62	2	269	76	1	0	30	6662
17.	* 9	000137-07-5	120453	29	75	2	55	78	1	1	30	5309
18.	* 9	060416-19-5	9430	28	64	3	292	75	1	0	33	5543
19.	9	000000-00-0	2210	45	68	1	45	80	1	0	35	4043
20.	* 9	004225-42-7	9117	42	53	1	99	74	1	5	30	7720



Peak 27
Extensive Subtraction to remove Peak 26 and Peak 28 from spectrum.



Scan 408 (11.806 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1180	57.00	193	79.05	337	121.05	54
43.85	228	57.90	237	80.00	145	122.05	57
46.90	17	61.90	57	81.00	413	124.05	1495
48.95	262	63.00	72	82.00	1276	125.95	106
50.00	412	66.00	258	82.95	14		
50.95	337	67.00	630	91.10	92		
52.00	141	68.00	127	92.95	141		
52.95	918	69.05	80	94.20	101		
54.05	1516	70.00	22	95.00	572		
55.05	270	77.00	109	96.05	258		
55.95	44	78.05	132	109.00	1321		

ethyl likely.

Compounds from Proctor and Gamble A0331.D

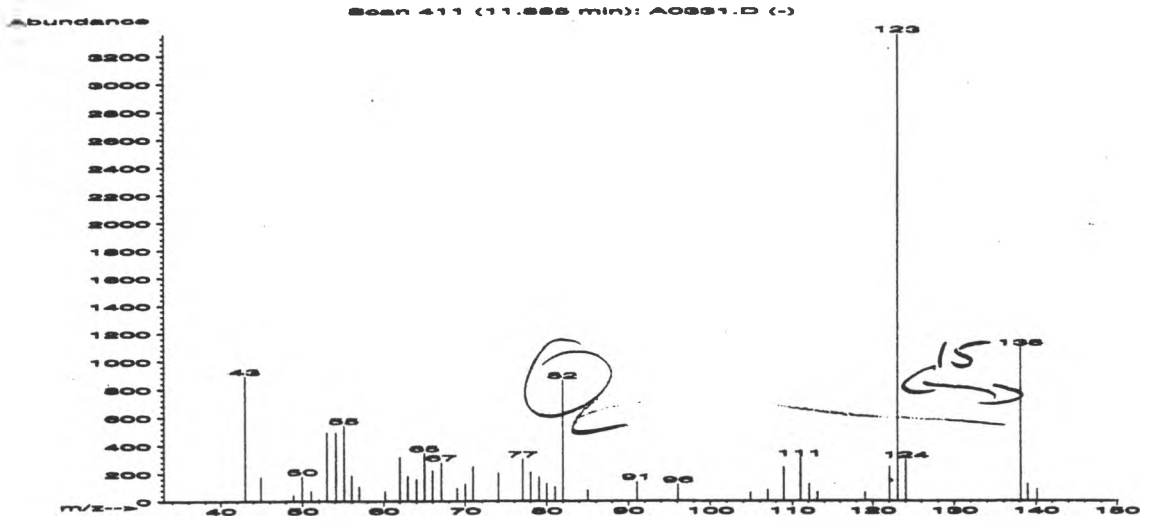
Scan 408 (11.806 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2H-Azepin-2-one, 1,5,6,7-tetrahydro-	111	C6H9NO	59
2.	2-Cyclohexen-1-one, 4,4-dimethyl-	124	C8H12O	43
3.	2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	42
4.	2-Norcaranone, 3-methyl-	124	C8H12O	42
5.	Thiophene, 2,5-dihydro-, 1,1-dioxide	118	C4H6O2S	38
6.	1,5-Cyclooctadiene, (E,Z)-	108	C8H12	35
7.	2-HYDROXY-4,6-DIMETHYLPYRIMIDINE-HYDROCH	124	C6H8N2O	25
8.	5,6-Dimethyl-2-pyrone	124	C7H8O2	22
9.	6,6-DIMETHYL-SPIRO[2.3]HEXAN-4-ONE	124	C8H12O	17
10.	2-Pentenenitrile	81	C5H7N	16
11.	2-Methyl -1-(ethylamino)-1-cyanopropene	124	C7H12N2	12
12.	Phenol, 2-methoxy-	124	C7H8O2	10
13.	2-Hexyne	82	C6H10	10
14.	2H-Pyran-2-one, 4,6-dimethyl-	124	C7H8O2	10
15.	2-(1-METHYLVINYL)THIOPHENE	124	C7H8S	9
16.	1,2-Heptadiene	96	C7H12	9
17.	3,6-DIMETHYL-2H-PYRAN-2-ONE	124	C7H8O2	9
18.	1-Pentyn-3-one, 4-methyl-	96	C6H8O	9
19.	2,4-Heptadiene, 2,4-dimethyl-	124	C9H16	8
20.	Ethanone, 1-(2-methyl-1-cyclopenten-1-yl	124	C8H12O	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	59	002228-79-7	2356	45	52	1	84	24	33	1	38	7253
2.	*43	001073-13-8	120411	51	64	2	93	48	18	20	47	7653
3.	*42	001123-09-7	4799	30	62	3	551	27	17	0	33	5922
4.	*42	029750-22-9	4829	46	75	2	98	28	17	11	33	8935
5.	38	000077-79-2	3717	39	65	0	98	40	14	2	35	5742
6.	35	005259-71-2	1986	44	43	1	99	54	11	18	38	5391
7.	*25	000108-79-2	120352	37	66	2	98	53	7	0	35	6709
8.	*22	004209-44-3	4696	42	64	2	98	65	5	0	39	6029
9.	*17	000000-00-0	4817	31	88	3	190	54	3	0	29	6672
10.	*16	013284-42-9	116729	28	56	0	78	57	3	2	35	5447
11.	*12	000000-00-0	4738	33	69	2	317	62	2	0	30	6368
12.	*10	000090-05-1	120379	43	54	0	68	78	1	5	40	6689
13.	*10	000764-35-2	116760	31	72	2	80	65	1	2	29	6365
14.	*10	000675-09-2	120364	44	75	3	167	77	1	0	40	5709
15.	* 9	030616-73-0	4734	35	58	0	88	80	1	2	35	6426
16.	* 9	002384-90-9	117600	31	62	3	169	73	1	0	33	5888
17.	* 9	053034-20-1	4694	29	87	2	82	80	1	1	30	7208
18.	* 9	013531-82-3	580	38	74	1	68	72	1	0	35	4841
19.	* 8	074421-05-9	4891	28	86	3	278	66	1	0	27	5903
20.	* 8	003168-90-9	4790	31	72	2	113	67	1	0	29	5983

Peak 28



Scan 411 (11.855 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	891	60.15	71	77.05	302	109.00	245
44.95	174	62.00	314	78.05	209	111.00	309
48.90	45	62.95	184	79.05	177	112.10	122
49.95	178	64.00	158	80.00	127	113.15	66
51.00	75	65.00	345	81.00	104	119.05	63
51.95	15	66.00	222	82.00	862	122.05	248
52.95	490	67.05	278	85.00	80	123.05	3351
54.05	490	69.00	96	91.05	139	124.05	297
55.05	543	70.05	126	96.05	119	138.10	1095
55.95	185	70.95	250	104.90	63	139.00	126
56.95	107	74.05	204	107.00	80	140.15	89

Compounds from Proctor and Gamble A0331.D

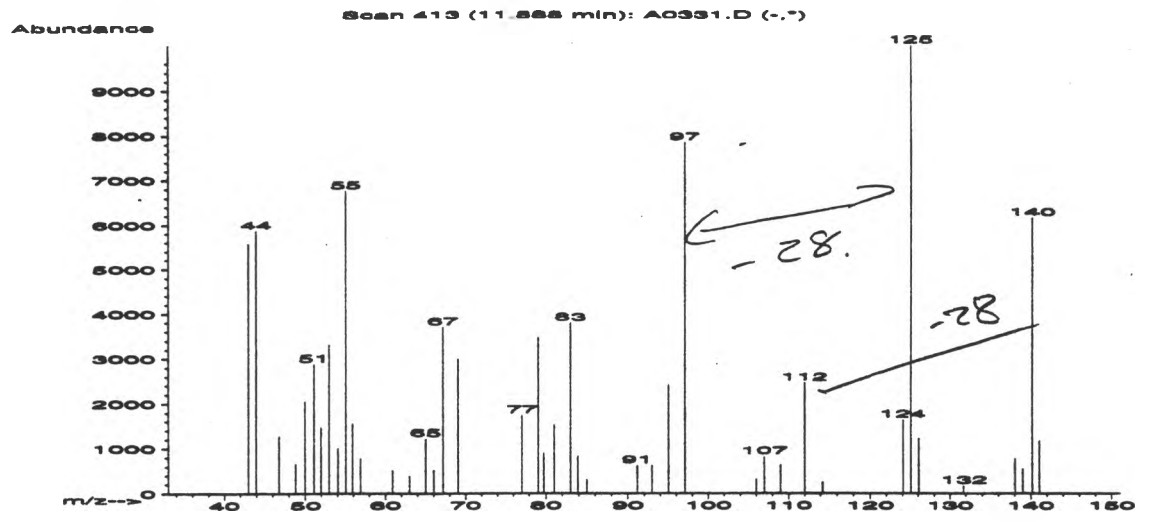
Scan 411 (11.855 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	4-Fluorocumene	138	C9H11F	64
2.	Benzene, 1,4-dimethoxy-	138	C8H10O2	46
3.	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	43
4.	2,2-Dimethyl-1-isopropenyl-cyclopentane	138	C10H18	43
5.	Cyclopentene, 1,3-dimethyl-2-(1-methylet	138	C10H18	43
6.	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	43
7.	Ethanone, 1-(4-fluorophenyl)-	138	C8H7FO	43
8.	3,3-Dimethyl-2-isopropyl-cyclopentene	138	C10H18	43
9.	Benzene, 1,4-dimethoxy-	138	C8H10O2	43
10.	Phenol, 4-amino-2-methyl-	123	C7H9NO	40
11.	Ethanone, 1-(3-fluorophenyl)-	138	C8H7FO	37
12.	Ethanone, 1-(4-fluorophenyl)-	138	C8H7FO	37
13.	Pyridine, 3-ethyl-, 1-oxide	123	C7H9NO	35
14.	2-(2-METHYLCYCLOPROPYL)THIOPHENE	138	C8H10S	27
15.	Benzenamine, 3-methoxy-	123	C7H9NO	27
16.	2(1H)-Pyridinone, 1,3-dimethyl-	123	C7H9NO	25
17.	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	25
18.	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	22
19.	2,5-Heptadien-4-one, 2,6-dimethyl-	138	C9H14O	17
20.	4-Pyrimidinamine, 2,6-dimethyl-	123	C6H9N3	17

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	000403-39-4	8585	29	23	1	96	18	37	9	42	9533
2.	*46	000150-78-7	8524	35	46	0	72	43	20	18	43	8956
3.	*43	002896-60-8	122223	35	58	1	73	43	18	5	40	9561
4.	*43	072535-87-6	122301	44	39	1	71	42	18	3	38	9741
5.	*43	061142-32-3	8767	42	36	0	74	43	18	11	40	9771
6.	*43	002896-60-8	8504	39	47	0	94	42	18	0	39	9606
7.	*43	000403-42-9	122215	33	59	1	99	41	18	0	39	9596
8.	*43	072535-89-8	8768	33	63	2	99	41	18	0	39	9742
9.	*43	000150-78-7	122245	45	42	0	85	42	18	12	40	8939
10.	*40	002835-96-3	4588	31	54	1	99	35	16	1	30	8900
11.	*37	000455-36-7	8474	39	60	1	99	41	13	0	33	9606
12.	*37	000403-42-9	8475	29	46	0	85	43	13	5	35	9553
13.	*35	014906-62-8	4553	35	62	1	72	55	11	0	39	9131
14.	*27	087688-54-8	8563	43	64	2	64	57	8	0	40	9604
15.	*27	000536-90-3	4583	33	56	2	99	56	8	0	39	9119
16.	*25	006456-92-4	4560	33	68	1	78	53	7	0	35	9144
17.	*25	000461-98-3	120304	35	48	1	99	51	7	3	36	9297
18.	*22	000615-05-4	8465	35	61	1	65	64	5	0	39	9490
19.	17	000504-20-1	122262	40	58	1	68	53	3	0	29	9387
20.	*17	000461-98-3	4540	31	62	1	75	52	3	0	29	9276

Peak 29



Scan 413 (11.888 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	5569	56.90	780	83.00	3785	114.25	255
43.95	5866	60.90	511	83.90	831	124.05	1640
46.80	1268	63.00	390	85.00	311	125.05	10000
48.80	655	65.00	1222	91.15	618	126.05	1226
49.95	2048	66.00	520	92.95	627	131.75	163
51.05	2875	67.15	3693	95.05	2411	138.05	771
51.95	1472	69.05	2987	97.05	7831	139.00	543
52.95	3312	77.05	1732	106.00	311	140.15	6140
54.05	1013	79.05	3456	107.00	813	141.05	1166
55.05	6758	79.75	887	109.00	632		
55.90	1556	81.00	1519	112.00	2457		

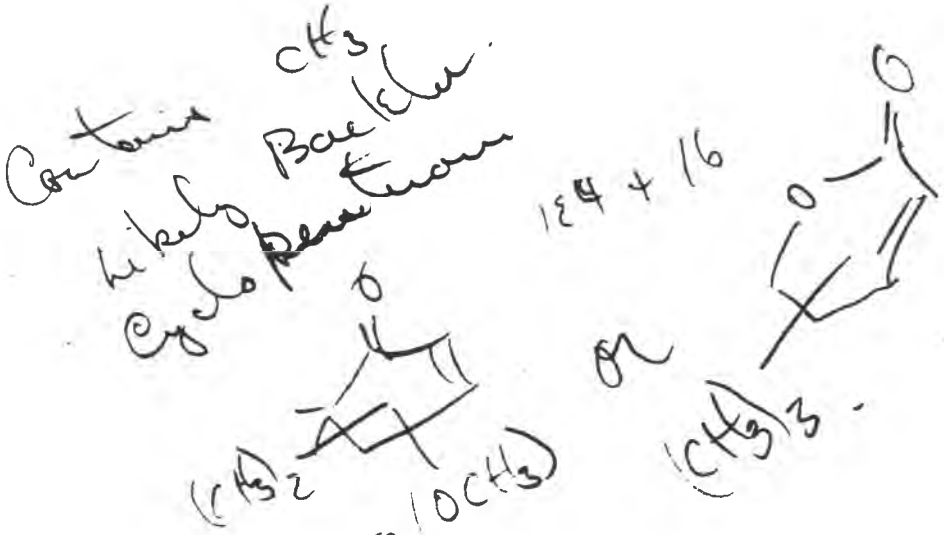
Compounds from Proctor and Gamble A0331.D

Scan 413 (11.888 min): A0331.D

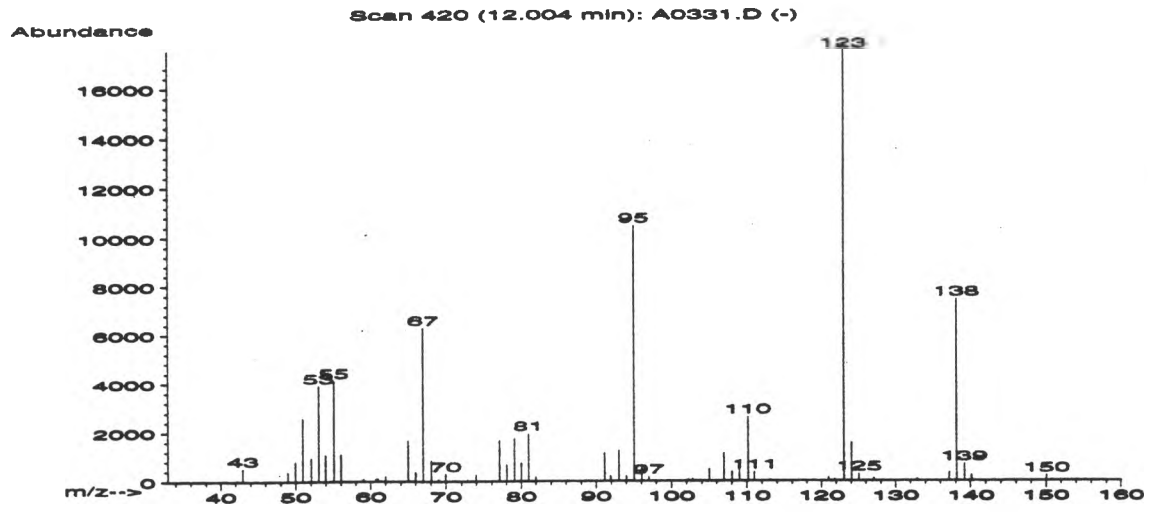
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	4-METHYL-5-VINYLTHIAZOLE	125	C6H7NS	46
2.	1-METHOXY-6,6-DIMETHYLCYCLOHEXENE	140	C9H16O	38
3.	2-ETHYL-3-METHOXY-2-CYCLOPENTENONE	140	C8H12O2	38
4.	Cyclohexanone, 2-acetyl-	140	C8H12O2	38
5.	1,3-Cyclopentanedione, 2-acetyl-	140	C7H8O3	35
6.	trans-2-Ethyl-3-methylcylohexanone	140	C9H16O	27
7.	m-Menthane, (1S,3R)-(+)-	140	C10H20	27
8.	Pyridinium, 3-mercapto-1-methyl-, hydrox	125	C6H7NS	22
9.	2-AMINO-5-METHYL-4-OXO-3,4-DIHYDROPYRIMI	125	C5H7N3O	22
10.	1-(ETHYL-1-D)-2-PYRIDONE	123	C7H7D2NO	22
11.	Cyclohexanone, dimethylhydrazone	140	C8H16N2	18
12.	Cyclohexane, 1,2-dimethyl-, cis-	112	C8H16	18
13.	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	18
14.	Pyridine, 3-(methylthio)-	125	C6H7NS	14
15.	ISONICOTINIC ACID-.BETA.-D2	123	C6H3D2NO2	14
16.	Cyclohexane, 1,4-dimethyl-, trans-	112	C8H16	14
17.	Cyclohexanone, dimethylhydrazone	140	C8H16N2	14
18.	Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	14
19.	M-TRIDEUTERIOMETHOXYTOLUENE	122	C8H7D3O	14
20.	4-Hydroxymethyl-hex-4-ene-1-ol	130	C7H14O2	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	001759-28-0	4965	47	71	0	94	43	20	0	44	8092
2.	*38	073741-66-9	9396	44	70	2	99	50	14	0	40	7970
3.	*38	025112-86-1	9267	43	79	1	73	46	14	0	40	8721
4.	*38	000874-23-7	9238	39	57	0	77	46	14	13	40	8776
5.	*35	003859-39-0	9106	37	62	2	83	53	11	12	40	7413
6.	27	075731-83-8	9393	44	33	0	75	58	8	0	39	5814
7.	*27	013837-66-6	9509	45	57	0	67	56	8	11	40	6028
8.	*22	036880-58-7	4972	34	68	1	81	63	5	11	40	6536
9.	*22	015981-91-6	4948	36	74	2	97	62	5	0	39	7360
10.	*22	053907-48-5	4558	45	52	0	76	64	5	14	43	6601
11.	*18	010424-93-8	122462	43	67	0	58	66	3	0	44	6618
12.	*18	002207-01-4	119111	37	62	0	54	68	3	3	43	5153
13.	*18	006876-23-9	2723	37	61	0	53	68	3	3	43	5158
14.	*14	018794-33-7	4975	35	63	1	91	70	2	7	40	6411
15.	*14	055090-51-2	4523	48	66	2	82	67	2	0	39	6768
16.	*14	002207-04-7	2727	39	61	0	63	68	2	0	39	5158
17.	*14	010424-93-8	9303	37	74	0	59	66	2	0	41	6710
18.	*14	000638-04-0	2724	33	64	0	71	68	2	0	41	5164
19.	*14	053884-73-4	4416	41	51	0	69	66	2	0	39	6412
20.	14	058203-49-9	6455	44	55	0	70	68	2	13	41	5093



Peak 30



Scan 420 (12.004 min): A0331.D

Scan 420 (12.004 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	530	61.00	110	78.05	689	97.00	167
48.95	380	62.00	212	79.05	1754	102.20	48
49.95	807	65.00	1665	80.00	753	102.80	77
50.95	2577	66.00	371	81.00	1950	105.00	494
52.05	962	67.00	6278	82.00	180	107.00	1149
53.05	3906	68.05	848	91.10	1158	108.00	390
53.95	1078	69.00	69	91.95	213	109.00	497
55.05	4123	69.95	292	93.05	1260	110.15	2620
56.00	1096	72.80	51	94.05	201	111.00	363
59.00	111	73.95	261	95.05	10450	113.15	48
60.75	108	77.05	1684	96.05	623	120.95	138

Scan 420 (12.004 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
121.80	61						
123.05	17520						
124.05	1574						
125.05	283						
127.05	122						
132.90	84						
137.15	343						
138.15	7460						
139.15	694						
140.15	232						
150.05	210						

Compounds from Proctor and Gamble A0331.D

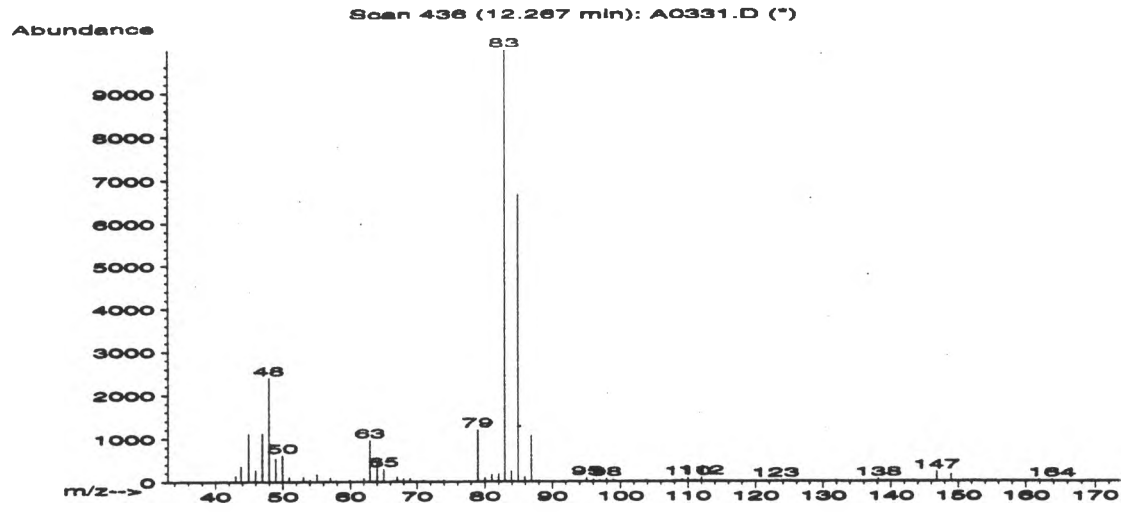
Scan 420 (12.004 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-Methoxy-4-methylphenol	138	C8H10O2	80
2.	2-Ethyl-2,5-dimethylcyclopent-2-enone	138	C9H14O	78
3.	3,3-Dimethyl-2-isopropyl-cyclopentene	138	C10H18	58
4.	Ethanone, 1-(4-fluorophenyl)-	138	C8H7FO	53
5.	Benzene, 1,4-dimethoxy-	138	C8H10O2	50
6.	Benzene, 1,4-dimethoxy-	138	C8H10O2	50
7.	Benzene, 1,4-dimethoxy-	138	C8H10O2	50
8.	3-ACETYL-2,5-DIMETHYLFURAN	138	C8H10O2	47
9.	4-ETHYL-3-METHYL-2H-PYRAN-2-ONE	138	C8H10O2	43
10.	2(1H)-Pyridinone, 1,3-dimethyl-	123	C7H9NO	43
11.	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	43
12.	2-Propanone, 1-(1-cyclohexen-1-yl)-	138	C9H14O	35
13.	Cyclohexene, 1-methyl-3-(1-methylethyl)-	138	C10H18	35
14.	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	30
15.	2,6-DIMETHYL-4-PYRIDINOL	123	C7H9NO	27
16.	1,4-Hexadiene, 2,3-dimethyl-	110	C8H14	25
17.	2,4-Hexadiene, 3,4-dimethyl-, (Z,Z)-	110	C8H14	25
18.	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	22
19.	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	14
20.	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	000093-51-6	8514	59	49	3	99	15	48	28	46	8936
2.	*78	096862-89-4	8609	49	21	1	82	9	46	19	39	9631
3.	*58	072535-89-8	8768	48	48	3	99	30	32	0	46	9438
4.	*53	000403-42-9	122215	51	37	3	99	26	28	10	39	9309
5.	*50	000150-78-7	8524	50	38	1	89	31	25	10	39	8733
6.	*50	000150-78-7	122245	49	44	2	97	31	25	6	40	8449
7.	*50	000150-78-7	122244	51	39	1	76	31	25	12	39	8981
8.	*47	000000-00-0	8487	35	39	1	74	36	20	0	41	8614
9.	*43	072185-10-5	8496	48	14	1	41	45	18	5	40	6095
10.	*43	006456-92-4	4560	36	65	2	99	45	18	0	41	8484
11.	*43	002896-60-8	122223	43	56	2	68	41	18	0	40	8655
12.	*35	000768-50-3	8638	35	63	2	59	55	11	18	40	6241
13.	*35	013828-31-4	8790	52	47	2	51	55	11	18	39	5283
14.	*30	000756-02-5	2255	62	26	0	44	63	9	0	56	5587
15.	*27	000000-00-0	4565	35	49	0	71	60	8	0	41	7792
16.	*25	018669-52-8	2242	36	35	0	44	65	7	2	43	5596
17.	*25	021293-01-6	2252	67	11	0	42	63	7	25	47	5442
18.	*22	000764-13-6	118889	62	14	1	45	65	5	19	39	5412
19.	*14	000764-13-6	118892	44	31	0	39	69	2	20	40	5319
20.	*14	000764-13-6	118891	44	31	0	39	69	2	20	40	5319

Peak 31



Scan 436 (12.267 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	129	55.05	161	69.95	17	86.90	1063
43.80	352	57.00	82	70.95	33	88.00	13
44.95	1094	57.90	24	73.95	38	95.05	83
45.95	260	59.90	34	78.95	1194	96.05	45
46.95	1093	62.00	69	80.00	79	96.95	32
47.95	2393	62.90	953	81.00	160	97.95	57
48.95	533	64.00	434	82.00	176	98.95	41
49.95	604	65.00	290	82.90	10000	103.95	25
50.95	97	67.00	103	83.90	246	109.15	40
53.05	108	67.95	53	84.90	6662	110.00	76
54.05	40	68.95	76	85.90	108	110.90	22

Scan 436 (12.267 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
112.00	91						
120.95	7						
122.95	30						
124.20	9						
125.05	23						
138.15	50						
146.80	219						
148.95	155						
161.90	31						
163.75	31						

Compounds from Proctor and Gamble A0331.D

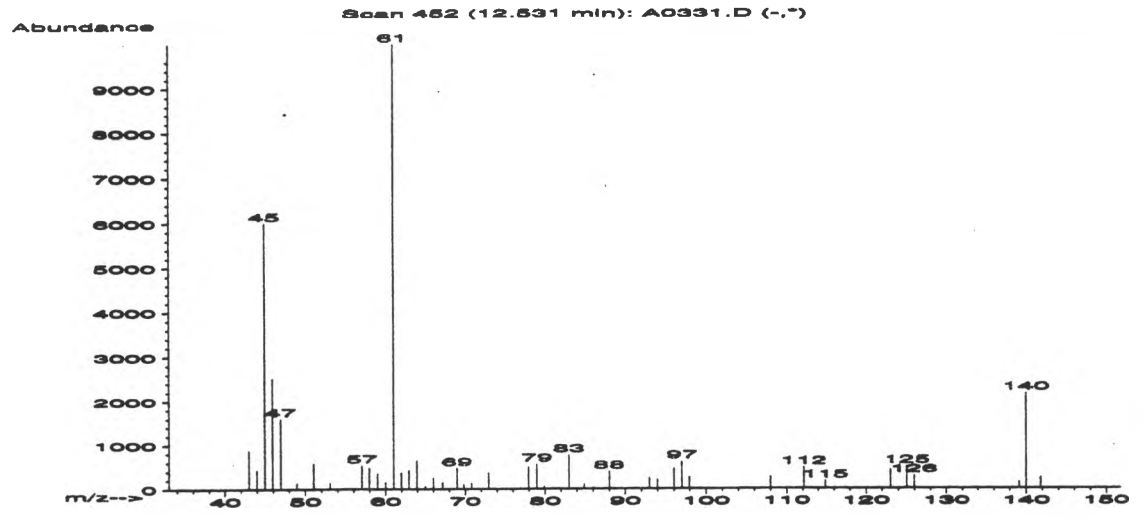
Scan 440 (12.333 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Dichloromethyl methyl sulfone	162	C2H4Cl2O2S	72
2.	TETRANEURIN - C	366	C19H26O7	59
3.	Ethane, 1,2,2-trichloro-1,1-difluoro-	168	C2HCl3F2	59
4.	Acetyl chloride, dichloro-	146	C2HCl3O	50
5.	Ethane, 2,2-dichloro-1,1,1-trifluoro-	152	C2HCl2F3	50
6.	Methane, bromodichloro-	162	CHBrCl2	50
7.	Methane, bromodichloro-	162	CHBrCl2	45
8.	Acetyl chloride, dichloro-	146	C2HCl3O	40
9.	Ethane, 1,1,2-trichloro-2-fluoro-	150	C2H2Cl3F	38
10.	Acetic acid, trichloro-	162	C2HCl3O2	38
11.	Chloroform	118	CHCl3	38
12.	Chloroform	118	CHCl3	38
13.	Pyrrolidine, 1-[8-(3-octyloxiranyl)-1-ox	351	C22H41NO2	38
14.	Chloroform	118	CHCl3	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	037557-96-3	17360	55	8	1	83	13	42	20	40	9839
2.	59	028587-46-4	91537	47	91	2	71	23	33	1	38	9835
3.	59	000354-21-2	125678	54	37	1	73	23	33	1	40	9806
4.	50	000079-36-7	123055	43	68	1	81	20	25	0	34	9675
5.	50	000306-83-2	123825	41	71	1	99	20	25	0	33	9873
6.	50	000075-27-4	17356	36	55	3	67	17	25	3	30	9882
7.	45	000075-27-4	125009	40	60	2	68	23	19	0	33	9850
8.	40	000079-36-7	123056	56	58	1	80	15	16	0	27	9475
9.	38	000359-28-4	12384	39	66	2	99	23	14	0	29	9775
10.	38	000076-03-9	125014	35	36	1	98	23	14	0	20	9650
11.	38	000067-66-3	119703	40	66	2	99	23	14	0	29	9690
12.	38	000067-66-3	3697	40	66	2	99	23	14	0	29	9690
13.	38	056630-37-6	134973	36	123	2	99	23	14	0	22	9606
14.	38	000067-66-3	119702	40	68	2	99	23	14	0	29	9665

Peak 32



Scan 452 (12.531 min): A0331.D

Modified:subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	881	60.00	143	72.95	359	96.00	458
43.95	432	61.00	10000	77.00	28	97.00	614
44.95	5993	61.95	359	77.95	495	97.95	257
45.95	2505	62.95	428	79.00	559	108.00	264
46.95	1594	63.95	649	79.95	57	112.15	476
48.95	136	65.00	64	83.00	768	114.90	168
51.05	577	66.00	260	84.90	108	123.05	425
53.05	134	67.15	147	86.05	27	125.05	497
57.00	531	68.95	467	88.00	391	125.95	290
57.95	479	69.80	97	92.95	242	139.15	145
59.00	347	70.80	129	93.95	205	140.00	2157

Scan 452 (12.531 min): A0331.D

Modified:subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
141.80	244						

Compounds from Proctor and Gamble A0331.D

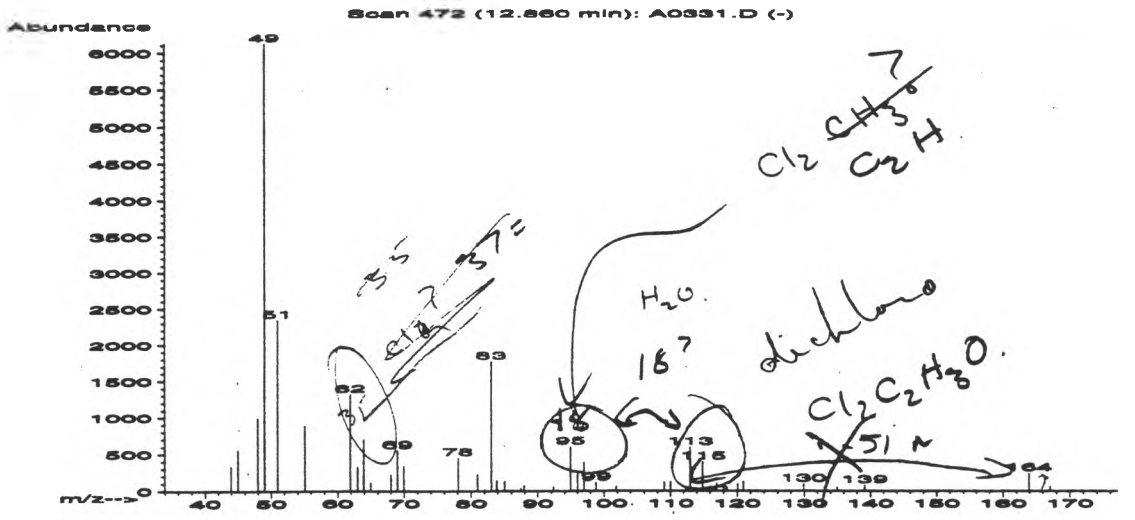
Scan 452 (12.531 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Disulfide, methyl (methylthio)methyl	140	C3H8S3	53
2.	Disulfide, methyl (methylthio)methyl	140	C3H8S3	53
3.	METHYL METHYLSULFINYLMETHYL SULFIDE	124	C3H8OS2	45
4.	2-(DIMETHYL PHOSPHINO)-ETHYL PHOSPHINE	122	C4H12P2	38
5.	Propanenitrile, 3-(methylthio)-	101	C4H7NS	28
6.	2,4-DITHIAPENTANE	108	C3H8S2	28
7.	2-(METHYLTHIO)ETHANOL	92	C3H8OS	12
8.	Disulfide, dimethyl	94	C2H6S2	12
9.	4-Oxo-1,2,4-trithiolane	140	C2H4OS3	10
10.	2-Octanol	130	C8H18O	7
11.	2-Octanol	130	C8H18O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	042474-44-2	122386	44	36	0	74	28	28	7	40	9574
2.	*53	042474-44-2	9001	44	36	0	74	28	28	7	40	9574
3.	45	033577-16-1	4621	45	61	3	88	21	19	0	37	9722
4.	38	054772-64-4	4302	36	100	2	99	23	14	0	22	9748
5.	28	054974-63-9	1266	34	76	0	97	38	8	0	25	9308
6.	28	001618-26-4	1853	34	80	1	80	38	8	0	22	9579
7.	12	005271-38-5	117413	37	72	2	55	58	2	0	20	9662
8.	12	000624-92-0	117490	39	62	2	46	58	2	0	29	6706
9.	*10	058966-90-8	8997	28	61	0	26	67	1	0	33	5238
10.	7	000123-96-6	6538	33	50	2	57	75	1	0	21	4963
11.	7	000123-96-6	121162	29	48	1	59	73	1	1	26	4958

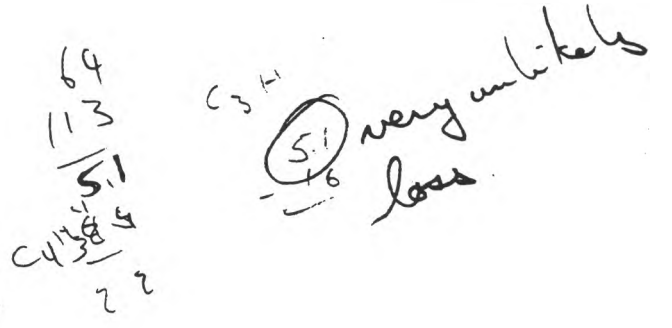
Peak 33



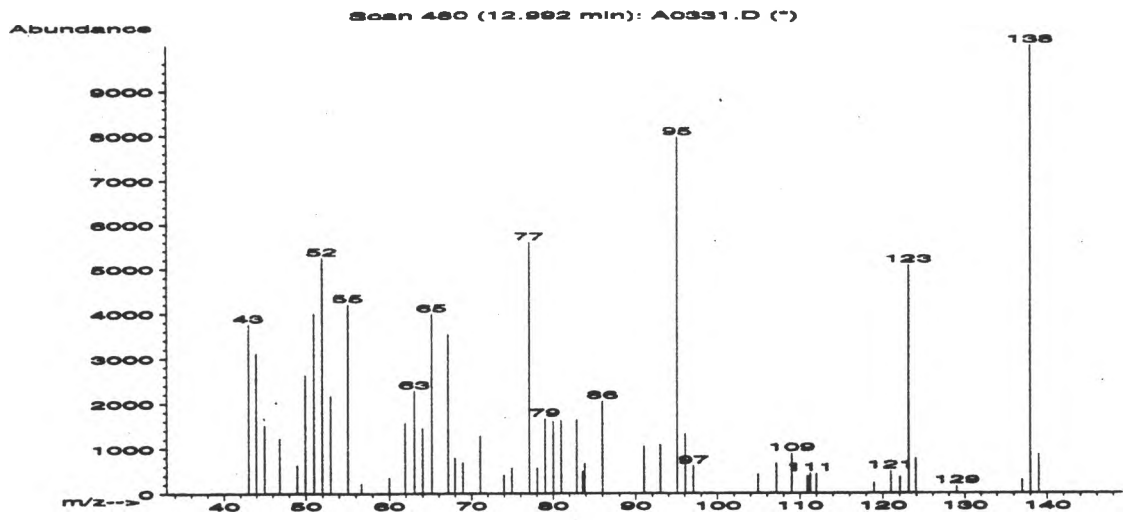
Scan 472 (12.860 min): A0331.D

Modified:subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	544	68.95	895	93.00	21	118.05	126
44.95	914	69.95	548	94.95	984	118.45	91
47.95	1618	78.05	739	96.00	379	120.05	155
48.95	10000	81.00	371	96.95	630	120.95	212
50.95	3830	82.00	31	98.80	181	129.90	153
55.05	1446	83.00	2897	101.80	100	135.00	78
61.90	2150	83.85	232	109.00	196	139.15	124
62.95	535	85.00	222	110.00	201	163.90	392
63.90	1148	87.40	57	113.00	973	167.05	100
64.95	181	87.90	119	114.90	648		
68.00	367	92.30	90	116.95	157		



Peak 34



Scan 480 (12.992 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	3757	60.00	354	77.05	5599	95.05	7945
43.95	3110	61.90	1565	78.05	567	96.05	1315
44.95	1512	63.00	2276	79.05	1658	97.05	607
46.80	1218	64.00	1448	80.00	1602	104.90	417
48.95	627	65.15	3987	81.00	1625	107.15	657
49.95	2623	67.15	3540	82.90	1635	109.00	891
50.95	3991	67.95	787	83.65	494	110.90	384
51.95	5245	68.95	687	83.90	661	111.25	440
52.95	2162	71.05	1278	86.00	2045	112.00	430
55.05	4198	73.95	414	91.00	1054	118.95	230
56.65	224	74.95	567	92.95	1081	120.95	494

Scan 480 (12.992 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	360						
123.05	5078						
123.95	764						
129.00	163						
137.00	304						
138.00	10000						
139.00	861						

Compounds from Proctor and Gamble A0331.D

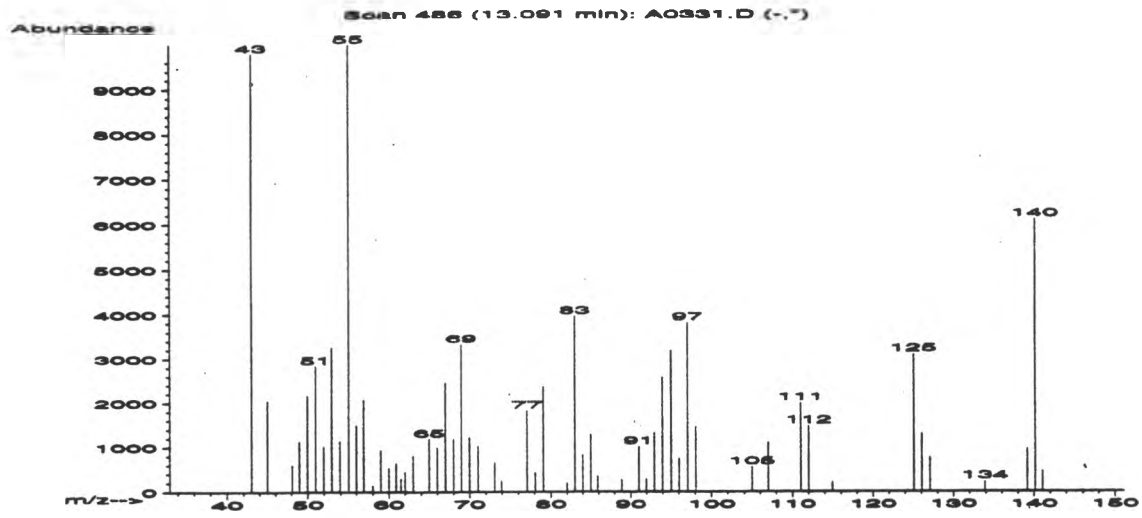
Scan 480 (12.992 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzene, 1,2-dimethoxy-	138	C8H10O2	96
2.	Benzene, 1,2-dimethoxy-	138	C8H10O2	95
3.	Benzene, 1,2-dimethoxy-	138	C8H10O2	95
4.	Benzene, 1,2-dimethoxy-	138	C8H10O2	81
5.	2-Methoxy-1,4-benzenediamine	138	C7H10N2O	59
6.	7-HYDROXYDISPIRO(2.0.2.2)OCTANE	124	C8H12O	40
7.	Benzoic acid, 3-hydroxy-	138	C7H6O3	38
8.	Benzenamine, 3-nitro-	138	C6H6N2O2	35
9.	2-Propenoic acid, 3-(2-furanyl)-	138	C7H6O3	25
10.	Benzeneethanamine, 4-methoxy-	151	C9H13NO	25
11.	2,5-Cyclohexadiene-1,4-dione, dioxime	138	C6H6N2O2	22
12.	Benzenamine, 2-nitro-	138	C6H6N2O2	22
13.	Benzenemethanol, 4-methoxy-	138	C8H10O2	16
14.	Copper chelate of 2-Nitrosophenol	123	C6H5NO2	16
15.	Benzene, 1,4-dimethoxy-	138	C8H10O2	12
16.	Dimethylphenylphosphine	138	C8H11P	10
17.	1,3-Benzodioxol-5-ol	138	C7H6O3	10
18.	Benzenemethanol, 4-methoxy-	138	C8H10O2	9
19.	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	9
20.	1,3-Benzodioxol-5-ol	138	C7H6O3	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000091-16-7	8522	103	19	0	92	4	76	57	96	9718
2.	*95	000091-16-7	122236	92	27	0	93	10	74	0	95	9801
3.	*95	000091-16-7	122238	106	20	0	81	10	74	49	95	9642
4.	*81	000091-16-7	122237	86	34	1	92	16	49	14	70	9544
5.	*59	000000-00-0	8466	35	46	2	81	23	33	0	39	8045
6.	40	064149-35-5	4852	47	80	3	91	33	16	0	34	7284
7.	*38	000099-06-9	122206	33	67	2	96	46	14	0	39	6372
8.	*35	000099-09-2	8415	33	71	0	81	51	11	18	38	6648
9.	*25	000539-47-9	8431	54	70	1	73	63	7	0	49	6369
10.	25	000055-81-2	13171	58	63	1	126	52	7	12	33	5759
11.	*22	000105-11-3	8419	33	64	2	97	63	5	5	40	6883
12.	*22	000088-74-4	122188	37	67	0	74	61	5	0	41	6951
13.	*16	000105-13-5	122235	38	87	3	88	58	3	1	36	7426
14.	*16	000000-00-0	4531	44	67	2	50	56	3	0	35	3804
15.	*12	000150-78-7	122242	42	66	3	99	61	2	2	31	7375
16.	*10	000672-66-2	122253	54	56	3	85	74	1	17	40	7446
17.	*10	000533-31-3	122212	36	68	0	98	73	1	0	41	6882
18.	* 9	000105-13-5	8521	39	81	2	81	78	1	0	35	7288
19.	* 9	000615-05-4	8465	36	68	2	172	74	1	0	30	6603
20.	* 9	000533-31-3	8440	34	75	1	99	72	1	0	35	6928

Peak 35



Scan 486 (13.091 min): A0331.D

Modified:subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	9796	56.90	2069	68.00	1181	84.00	819
44.95	2041	58.00	134	68.95	3328	85.00	1283
48.05	599	59.00	933	69.95	1218	85.90	350
48.95	1132	60.00	525	71.05	1026	88.90	273
49.95	2155	60.90	631	73.05	648	91.00	1010
50.95	2835	61.50	285	73.95	240	91.95	281
51.95	1022	62.00	436	77.05	1817	92.95	1320
52.95	3255	63.00	807	78.05	428	93.95	2578
53.95	1136	65.00	1181	79.05	2375	95.05	3185
55.05	10000	66.00	994	82.00	204	96.05	733
56.00	1491	67.00	2460	83.00	3955	97.05	3813

Scan 486 (13.091 min): A0331.D

Modified:subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.05	1458	139.15	953				
105.00	554	140.15	61147				
107.00	1104	141.05	444				
111.05	1996						
112.00	1479						
114.90	212						
125.05	3100						
126.05	1295						
127.05	766						
133.90	220						
138.05	4						

C_6H_5Cl

$C_7H_8O_3$

Scan 486 (13.091 min): A0331.D

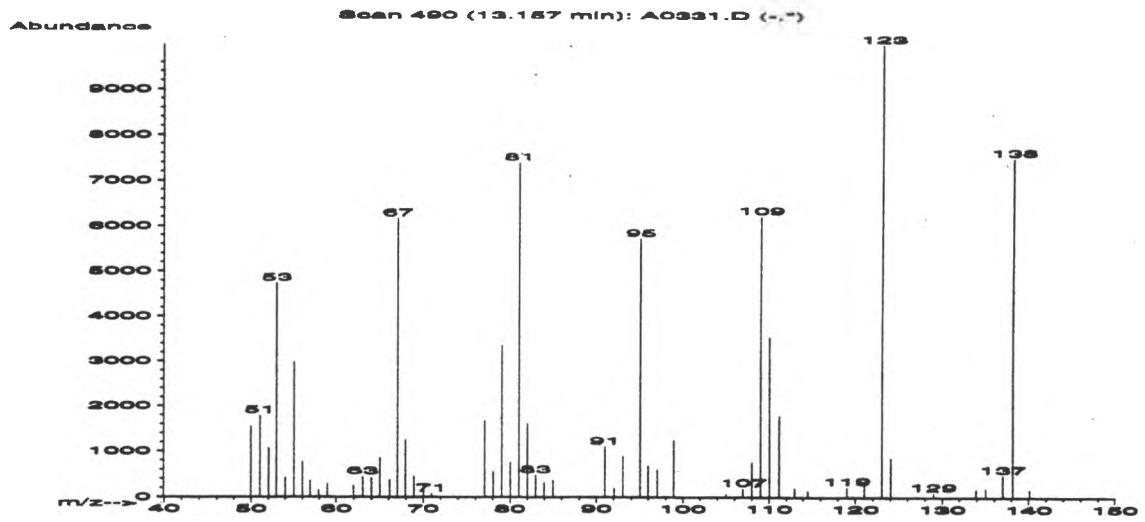
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3-t-Butyl-2-(5H)-furanone	140	C8H12O2	38
2.	CYCLODECANE	140	C10H20	32
3.	1,2,2,3-Tetramethyl-3-cyclopenten-1-ol	140	C9H16O	25
4.	3-Hexene, 2,2-dimethyl-, (E)-	112	C8H16	25
5.	1,4-Benzenediol, 2-methoxy-	140	C7H8O3	22
6.	2,4(1H,3H)-Pyrimidinedione, 1,3-dimethyl	140	C6H8N2O2	22
7.	4H-Pyran-4-one, 3-hydroxy-2,6-dimethyl-	140	C7H8O3	22
8.	1-Hexadecanol	242	C16H34O	16
9.	1,12-Tridecadien-7-one	194	C13H22O	14
10.	Uracil, 5-ethyl-	140	C6H8N2O2	14
11.	2-Nitro-2-(3'-hydroxybutyl)cyclooctanone	243	C12H21NO4	14
12.	Cyclohexanone, 2-acetyl-	140	C8H12O2	12
13.	17-Pentatriacontene	491	C35H70	12
14.	1-Nonene	126	C9H18	12
15.	2-Hexenal, 2-ethyl-	126	C8H14O	11
16.	3-Hexen-2-one, 3,4-dimethyl-, (Z)-	126	C8H14O	11
17.	1,3,5,7-Tetraazatricyclo[3.3.1.1(3,7)]de	140	C6H12N4	10
18.	2-Hexenal, 2-ethyl-	126	C8H14O	10
19.	3-Heptene, 4-methyl-	112	C8H16	10
20.	3-Hexen-2-one, 3,4-dimethyl-, (E)-	126	C8H14O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	063711-18-2	9195	41	51	0	41	48	14	3	38	8120
2.	32	000000-00-0	9539	55	67	2	37	46	9	0	36	7998
3.	25	074055-14-4	9371	46	69	1	76	53	7	0	35	7193
4.	*25	000690-93-7	119079	44	49	0	70	64	7	0	44	5383
5.	*22	000824-46-4	9120	39	51	0	41	61	5	6	39	7821
6.	*22	000874-14-6	122394	35	63	1	61	62	5	0	39	7331
7.	*22	002298-99-9	122425	34	49	1	95	64	5	0	39	7445
8.	16	036653-82-4	53510	47	102	3	90	60	3	15	35	6052
9.	14	054560-99-5	32028	44	69	3	96	70	2	1	38	5020
10.	*14	004212-49-1	9060	33	36	1	46	68	2	10	40	6851
11.	14	086911-18-4	53650	46	83	0	56	66	2	0	39	5856
12.	*12	000874-23-7	9238	35	74	2	109	64	2	11	37	6739
13.	12	006971-40-0	108269	58	109	2	57	63	2	0	36	6486
14.	12	000124-11-8	120614	57	62	3	97	64	2	0	36	5467
15.	*11	000645-62-5	120572	37	62	0	70	73	2	12	43	5333
16.	*11	020685-45-4	120590	49	53	0	97	71	2	0	46	5119
17.	*10	000100-97-0	122400	33	60	1	130	76	1	0	39	6314
18.	10	000645-62-5	120574	56	51	1	99	68	1	0	36	5304
19.	*10	004485-16-9	119063	33	56	0	79	80	1	0	41	4751
20.	*10	020685-46-5	5316	42	55	0	97	73	1	0	39	4411

Compounds from Proctor and Gamble A0331.D

Peak 36



Scan 490 (13.157 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.95	1535	63.00	440	79.05	3354	96.00	681
51.00	1789	64.00	410	80.00	759	97.05	595
52.00	1070	65.00	863	81.00	7374	98.95	1240
52.95	4732	66.10	372	82.00	1608	105.00	66
54.00	413	67.00	6153	83.00	478	107.00	187
55.00	2975	67.95	1250	83.95	313	108.00	759
56.00	766	68.95	449	85.00	361	109.00	6199
56.95	355	70.05	283	91.00	1100	110.05	3535
57.95	151	71.00	70	92.05	191	111.15	1770
58.95	291	77.05	1678	93.05	893	113.00	198
61.95	247	78.05	555	95.05	5712	114.50	134

Scan 490 (13.157 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.05	219						
121.05	259						
123.05	10000						
124.05	849						
129.00	89						
133.90	168						
135.00	193						
137.00	481						
138.15	7493						
140.10	166						

Compounds from Proctor and Gamble A0331.D

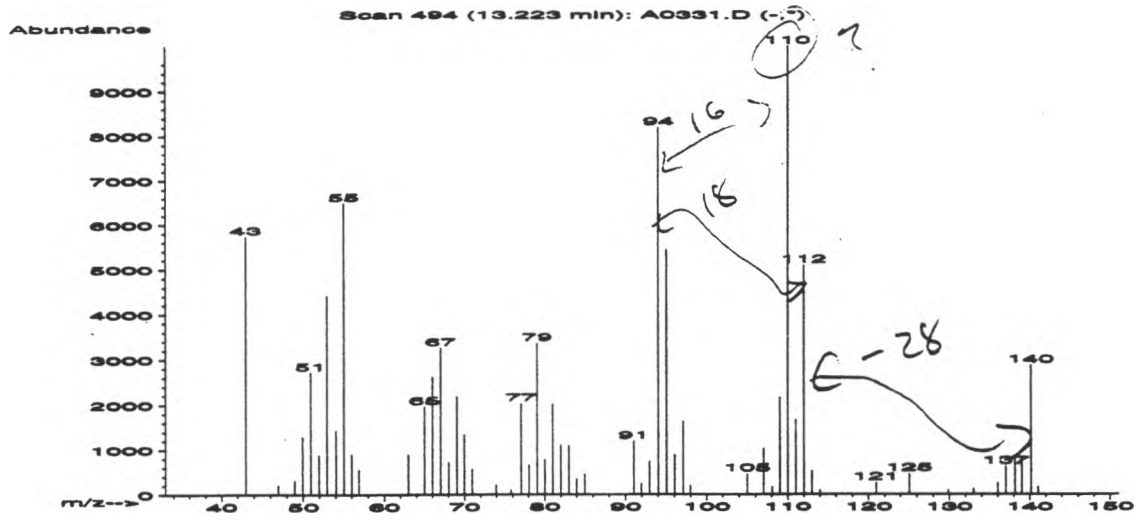
Scan 490 (13.157 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclohexene, 1-methyl-4-(1-methylethyl)-	138	C10H18	64
2.	2-Ethyl-2,5-dimethylcyclopent-2-enone	138	C9H14O	43
3.	3,4-Octadiene, 7-methyl-	124	C9H16	43
4.	Pulegone	152	C10H16O	38
5.	Cyclopropane, 1,1,2-trimethyl-3-(2-methy	138	C10H18	38
6.	Cyclooctene	110	C8H14	27
7.	1,4-Dimethylcyclohex-1-en-4-ylcarboxalde	138	C9H14O	27
8.	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	25
9.	Cyclohexanone, 2-(1-methylethylidene)-	138	C9H14O	22
10.	Benzene, 1,4-dimethoxy-	138	C8H10O2	18
11.	Cyclopropane, tetramethylmethylene-	110	C8H14	15
12.	1,3-Benzenediol, 4,5-dimethyl-	138	C8H10O2	14
13.	3-Octyne	110	C8H14	14
14.	2-Octyne	110	C8H14	14
15.	1,4-Heptadiene, 3-methyl-	110	C8H14	14
16.	2-Methoxy-4-methylphenol	138	C8H10O2	14
17.	Cyclopropane, 1,2-dimethyl-3-methylene-	82	C6H10	14
18.	Cyclopentene, 4,4-dimethyl-	96	C7H12	14
19.	trans-4,5-Dimethylcyclopent-2-en-1-one	110	C7H10O	11
20.	5-Dimethylamino-4-penten-2-ynal	123	C7H9NO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	029350-67-2	122304	64	61	1	60	24	37	24	46	7622
2.	*43	096862-89-4	8609	35	34	0	92	42	18	0	41	8032
3.	*43	037050-05-8	4880	55	56	2	109	46	18	0	47	6420
4.	38	000089-82-7	123986	64	32	2	70	50	14	15	40	5317
5.	*38	054764-57-7	8758	48	61	1	64	54	14	19	44	8806
6.	*27	000931-88-4	118908	44	53	2	49	57	8	0	40	5933
7.	*27	000933-44-8	8627	34	65	0	73	59	8	0	41	8164
8.	*25	000615-05-4	8465	50	48	1	99	61	7	0	44	7561
9.	*22	013747-73-4	8629	50	60	1	54	65	5	10	39	7260
10.	*18	000150-78-7	8524	46	47	2	91	67	3	0	44	7100
11.	*15	054376-39-5	2264	58	46	0	50	79	2	0	56	5485
12.	*14	000527-55-9	8505	44	59	2	74	69	2	0	40	6822
13.	*14	015232-76-5	118879	64	43	1	69	66	2	18	40	6283
14.	*14	002809-67-8	118877	49	54	2	53	69	2	18	39	6404
15.	*14	001603-01-6	2229	67	38	2	73	66	2	1	40	6592
16.	*14	000093-51-6	8514	45	60	1	67	66	2	0	39	7510
17.	*14	062338-02-7	116779	35	65	3	180	69	2	0	41	4024
18.	14	019037-72-0	638	43	49	3	197	68	2	0	39	4673
19.	*11	032556-65-3	2190	34	19	0	57	80	2	2	43	5074
20.	*10	080487-48-5	4544	45	66	1	74	80	1	0	40	6156

Peak 37



Scan 494 (13.223 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	5735	63.00	898	77.05	2029	92.95	740
46.95	209	64.00	24	78.05	661	94.05	8175
48.95	318	65.00	1952	79.05	3357	95.05	5436
49.95	1291	66.00	2610	80.00	782	96.05	886
50.95	2706	67.00	3247	81.00	2012	97.05	1627
51.95	886	68.05	724	82.00	1104	97.95	208
52.95	4400	69.05	2183	83.00	1087	105.00	459
54.05	1439	69.95	1344	84.00	351	107.00	1032
55.05	6482	70.95	566	85.00	463	108.10	171
56.00	902	73.95	222	91.00	1187	109.00	2157
56.90	554	75.80	103	91.95	247	110.00	10000

Scan 494 (13.223 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.00	1667	139.00	854				
112.00	5091	140.15	2870				
113.00	519	141.05	175				
114.00	95						
120.95	269						
125.05	470						
129.90	90						
133.00	131						
136.00	251						
137.00	624						
138.15	778						

Compounds from Proctor and Gamble A0331.D

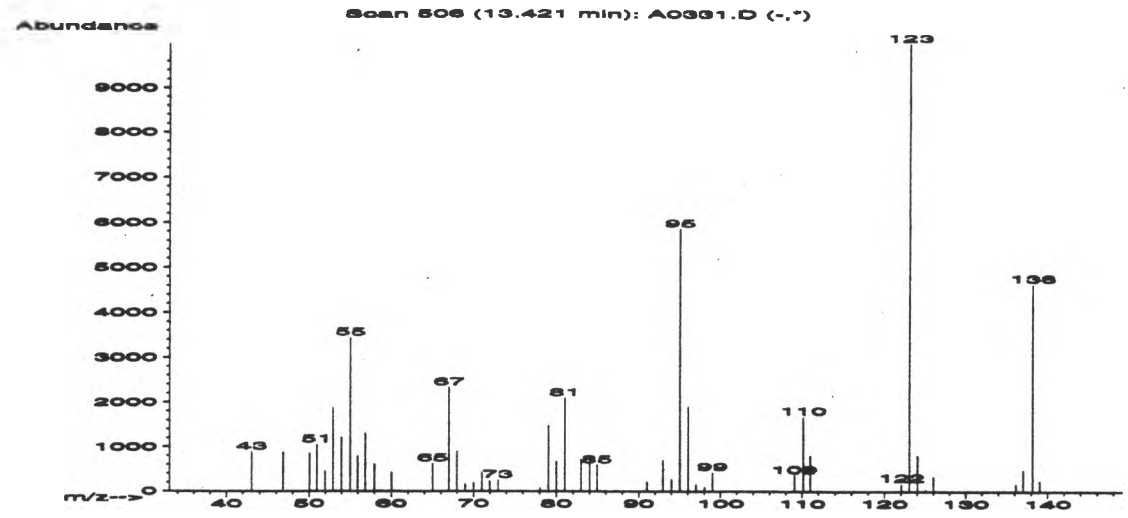
Scan 494 (13.223 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclopropane, tetramethylmethylene-	110	C8H14	35
2.	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	35
3.	2,4-Hexadiene, 3,4-dimethyl-, (Z,Z)-	110	C8H14	35
4.	2,4-Hexadiene, 3,4-dimethyl-, (E,Z)-	110	C8H14	35
5.	2-Methyl-1-(methylamino)-1-cyanopropene	110	C6H10N2	35
6.	3-HEPTYNE-2-ONE	110	C7H10O	22
7.	Benzenethiol	110	C6H6S	22
8.	Phenol	94	C6H6O	14
9.	Phenol	94	C6H6O	14
10.	Phenol	94	C6H6O	14
11.	Phenol	94	C6H6O	14
12.	3-Aminopyridine-N-oxide	110	C5H6N2O	12
13.	1,4-Benzenediol	110	C6H6O2	11
14.	1-Propene, 1,1-dichloro-	110	C3H4Cl2	11
15.	5-HYDROXY-2-PYRIDYL METHYL KETONE	137	C7H7NO2	11
16.	7-SYN-HYDROXY-BICYCLO[2.2.2]OCT-5-EN-2-O	138	C8H10O2	10
17.	Borazine, 2,4-dimethyl-	109	C2H10B3N3	10
18.	1H-Pyrrole, 2,5-dimethyl-	95	C6H9N	10
19.	7-ANTI-HYDROXY-BICYCLO[2.2.2]OCT-5-EN-2-	138	C8H10O2	10
20.	1H-Pyrrole, 2,5-dimethyl-	95	C6H9N	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	054376-39-5	2264	35	76	3	133	53	11	0	39	6375
2.	*35	000764-13-6	118890	34	72	2	160	52	11	0	39	6530
3.	*35	021293-01-6	2252	34	78	3	149	52	11	0	39	6591
4.	*35	002417-88-1	2253	34	77	3	126	51	11	0	39	7034
5.	*35	073171-64-9	2138	33	75	3	185	52	11	0	39	6486
6.	22	026059-43-8	2166	43	45	0	46	61	5	13	41	4252
7.	*22	000108-98-5	2135	47	63	1	91	63	5	0	40	6670
8.	*14	000108-95-2	117520	41	69	1	66	67	2	9	38	5572
9.	*14	000108-95-2	117519	33	51	0	81	68	2	0	41	5530
10.	*14	000108-95-2	117517	33	65	1	59	68	2	11	40	5673
11.	*14	000108-95-2	117515	33	58	1	72	69	2	0	41	5473
12.	*12	000000-00-0	2122	45	55	2	91	61	2	7	36	7702
13.	*11	000123-31-9	118840	43	49	0	89	79	2	0	44	6745
14.	*11	000563-58-6	2087	55	44	1	75	72	2	7	46	7056
15.	*11	067310-56-9	8249	37	52	0	67	74	2	4	43	6543
16.	*10	000000-00-0	8535	46	69	2	54	75	1	0	40	4695
17.	*10	023208-27-7	2022	37	72	0	41	72	1	0	41	5407
18.	*10	000625-84-3	532	35	56	1	76	76	1	0	39	6230
19.	*10	000000-00-0	8536	33	84	2	52	75	1	0	39	5002
20.	*10	000625-84-3	117543	34	64	1	81	76	1	0	39	6225

Peak 38



Scan 506 (13.421 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	888	60.00	417	80.00	674	98.05	98
46.80	881	65.00	623	81.00	2093	99.00	420
50.05	850	67.00	2324	83.00	718	109.05	359
50.95	1047	67.95	898	84.00	799	110.15	1677
51.95	447	68.95	159	84.90	589	111.00	803
52.95	1877	70.00	190	91.00	213	122.10	176
53.95	1209	71.00	420	93.00	691	123.05	10000
55.05	3428	71.95	230	94.00	261	124.05	806
55.95	789	72.95	247	95.05	5850	125.05	41
56.90	1301	78.05	78	96.05	1897	126.00	325
58.00	603	79.05	1484	97.00	156	136.15	163

Scan 506 (13.421 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.00	474						
138.15	4641						
139.05	237						

Compounds from Proctor and Gamble A0331.D

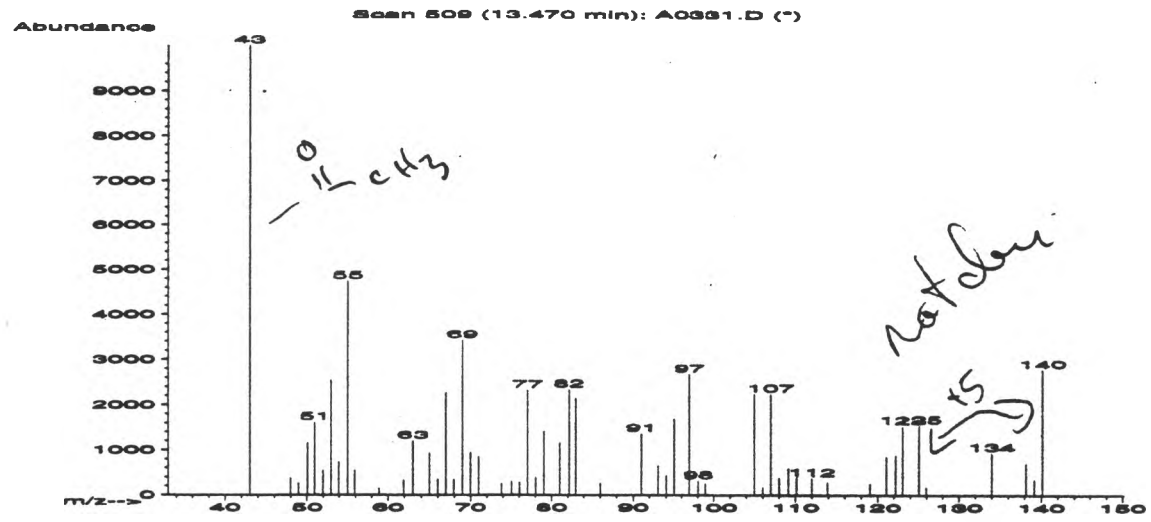
Scan 506 (13.421 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1,3-Benzenediamine, 4-methoxy-	138	C7H10N2O	83
2.	2-Ethyl-2,5-dimethylcyclopent-2-enone	138	C9H14O	72
3.	CYCLOPENTENE, 2-ISOPROPYL-3,4-DIMETHYL-	138	C10H18	64
4.	Cyclopentene, 1-isopropyl-4,5-dimethyl-	138	C10H18	64
5.	3-Methoxy-1,2-benzenediamine	138	C7H10N2O	64
6.	1,3-Benzenediol, 4-ethyl-	138	C8H10O2	58
7.	2-Methoxy-4-methylphenol	138	C8H10O2	53
8.	2,2-Dimethyl-1-isopropenyl-cyclopentane	138	C10H18	52
9.	4-ETHOXYPYRIDINE	123	C7H9NO	47
10.	3-ACETYL-2,5-DIMETHYLFURAN	138	C8H10O2	47
11.	1-Butanone, 4-chloro-1-(4-fluorophenyl)-	200	C10H10ClFO	45
12.	Furan, 2-(1,1-dimethylethyl)-4-methyl-	138	C9H14O	38
13.	4,4-Dimethyl-5-ethylcyclopent-2-en-1-one	138	C9H14O	38
14.	Phenol, 2-amino-5-methyl-	123	C7H9NO	27
15.	Phenol, 3-amino-2-methyl-	123	C7H9NO	27
16.	Cyclopentane, (3-methylbutylidene)-	138	C10H18	25
17.	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	25
18.	CYCLOHEXENE, 1,3-DIMETHYL-	110	C8H14	25
19.	2,4-Hexadiene, 2,5-dimethyl-	110	C8H14	25
20.	Pyridine, 3-ethyl-, 1-oxide	123	C7H9NO	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	000615-05-4	8465	70	39	1	91	11	50	18	53	9766
2.	*72	096862-89-4	8609	43	27	2	88	13	42	3	38	9677
3.	*64	000000-00-0	8769	48	50	1	74	20	37	17	39	8174
4.	*64	007712-74-5	8766	48	50	1	74	20	37	17	39	8174
5.	*64	000000-00-0	8464	46	22	1	94	18	37	11	40	9566
6.	*58	002896-60-8	8504	44	46	1	99	30	32	0	44	8960
7.	*53	000093-51-6	8514	35	64	2	80	27	28	13	40	9087
8.	*52	072535-87-6	122301	37	54	3	99	34	27	13	43	8922
9.	*47	033399-46-1	4570	46	41	1	71	39	20	20	43	8721
10.	*47	000000-00-0	8487	35	39	1	79	39	20	0	39	8738
11.	45	003874-54-2	34543	43	66	2	99	22	19	0	37	9619
12.	38	006141-68-0	8606	43	48	2	87	50	14	4	38	8736
13.	*38	081825-20-9	8610	47	60	2	64	36	14	11	36	8157
14.	*27	002835-98-5	4587	33	69	1	99	57	8	0	39	7775
15.	*27	053222-92-7	4586	34	62	0	99	60	8	0	41	7776
16.	*25	053366-51-1	8775	33	67	2	56	52	7	2	37	5306
17.	*25	000756-02-5	118896	35	51	1	50	64	7	14	43	4967
18.	*25	000000-00-0	2280	35	53	0	58	64	7	2	43	5095
19.	*25	000764-13-6	2251	34	42	0	39	65	7	16	43	4977
20.	*22	014906-62-8	4553	33	44	1	76	61	5	3	38	7826

Peak 39



Scan 509 (13.470 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	10000	61.90	330	76.05	278	95.05	1681
47.95	376	63.00	1203	77.05	2325	96.95	2675
48.95	263	65.00	936	78.05	397	98.05	311
50.05	1147	66.00	353	79.05	1420	98.95	257
50.95	1614	67.00	2270	81.00	1161	105.00	2239
51.95	547	67.95	340	82.15	2339	106.00	173
52.95	2540	68.95	3419	83.00	2143	107.00	2241
53.95	735	69.95	940	86.00	269	108.00	376
55.05	4737	70.95	848	91.00	1362	109.15	597
55.90	543	73.80	246	93.05	643	110.15	378
58.90	146	75.05	299	94.05	430	112.00	374

Scan 509 (13.470 min): A0331.D

Modified:scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
113.90	284						
119.05	246						
121.05	850						
122.20	879						
123.05	1529						
125.05	1548						
125.95	175						
134.00	936						
138.15	698						
139.15	334						
140.15	2778						

Compounds from Proctor and Gamble A0331.D

Scan 509 (13.470 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

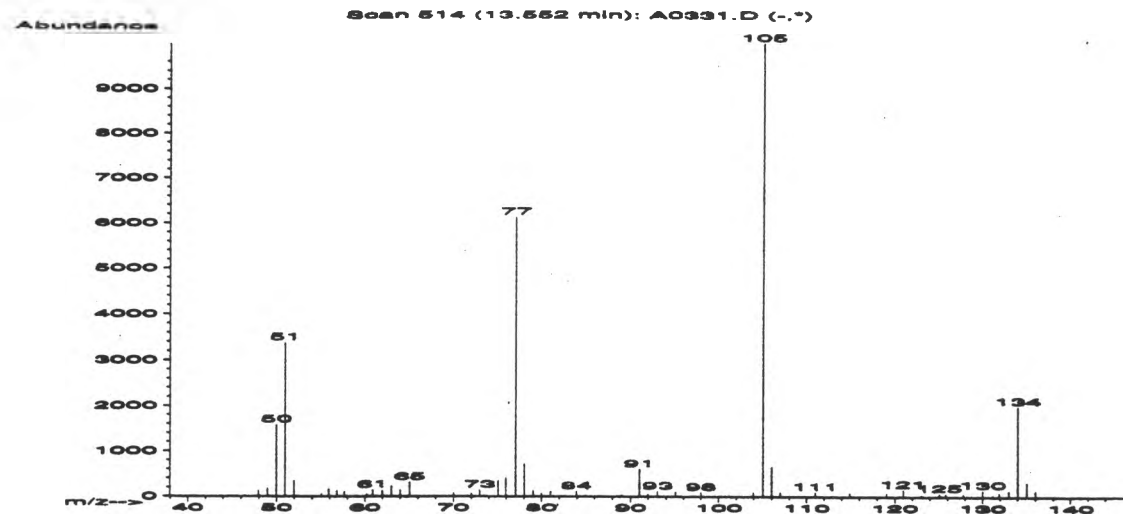
	Name	MolWt	Formula	Qual
1.	1,2,2,3-Tetramethyl-3-cyclopenten-1-ol	140	C9H16O	25
2.	8-Acetyl-3,3-epoxymethano-6,6,7-trimethy	236	C14H20O3	25
3.	2,11-Dodecanedione	198	C12H22O2	22
4.	2-Acetyl-4-nitrocyclononanone	227	C11H17NO4	12
5.	3-n-Amylcyclooctanone	196	C13H24O	10
6.	3-Pentyn-2-one, 5,5-diethoxy-	170	C9H14O3	10
7.	Octadecanal	268	C18H36O	10
8.	ETHYLDIPROPYL-BORANE	126	C8H19B	10
9.	17-Pentatriacontene	491	C35H70	9
10.	9-Octadecen-1-ol, (Z)-	268	C18H36O	9
11.	3-Octen-2-one, 7-methyl-	140	C9H16O	7
12.	PHOTOCITRAL B	152	C10H16O	7
13.	Decanal	156	C10H20O	7
14.	LONGIPINENEPOXIDE	220	C15H24O	7
15.	1-Azabicyclo[2.2.2]octan-3-one	125	C7H11NO	7
16.	1-Hexacosanol	382	C26H54O	7
17.	ISO-PINOCAMPHEOL	154	C10H18O	7
18.	3-Heptyn-2-ol	112	C7H12O	7
19.	1-Propanesulfonic acid, methyl ester	138	C4H10O3S	7
20.	2-METHOXY-13C-3-METHYLPYRAZINE	124	C513CH8N2O	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	25	074055-14-4	9371	45	53	1	40	53	7	0	35	7544
2.	25	091186-43-5	50791	54	78	3	99	55	7	8	34	8134
3.	22	007029-09-6	33921	60	74	1	30	62	5	0	39	6789
4.	12	086572-34-1	47086	43	61	1	88	65	2	8	33	6453
5.	10	084002-76-6	33120	37	20	0	71	65	1	0	25	5988
6.	10	055402-04-5	21273	33	63	1	71	65	1	1.	23	6088
7.	10	000638-66-4	132074	43	87	2	82	79	1	7	38	5711
8.*	10	000000-00-0	5406	29	61	0	77	70	1	0	33	5619
9.	9	006971-40-0	108269	41	113	2	80	74	1	4	35	5970
10.	9	000143-28-2	132077	45	101	3	57	72	1	0	31	5919
11.	7	033046-81-0	9336	34	68	2	99	77	1	0	22	5499
12.	7	055253-27-5	13633	37	47	1	51	79	1	0	22	4265
13.	7	000112-31-2	124506	39	84	2	53	79	1	0	29	4401
14.	7	000000-00-0	44059	33	98	3	136	79	1	0	21	4474
15.*	7	003731-38-2	5017	29	60	1	27	77	1	0	29	5021
16.	7	000506-52-5	94731	33	129	3	87	79	1	0	21	5668
17.	7	027779-29-9	124349	34	74	3	93	77	1	0	21	4825
18.*	7	056699-62-8	2577	31	68	1	43	79	1	0	26	5050
19.*	7	002697-50-9	8367	31	70	2	98	79	1	0	26	5718
20.	6	034061-82-0	4673	36	171	3	58	79	1	0	13	4846

$C_8H_{12}O_2$

96
32
3/8
12

Peak 40



Scan 514 (13.552 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
47.95	129	60.90	139	77.05	6120	95.05	95
48.95	175	62.00	128	78.05	718	98.00	88
49.95	1570	63.00	231	79.05	131	103.95	81
50.95	3371	64.00	137	80.00	59	105.00	10000
51.95	345	65.05	308	81.00	101	106.00	662
55.05	51	66.10	13	83.95	111	107.00	90
55.90	169	70.00	75	85.00	27	111.00	99
56.80	119	72.00	60	89.00	40	114.90	85
57.65	106	72.95	142	91.00	606	119.05	75
59.00	18	75.05	348	91.95	50	120.95	152
60.25	47	75.95	407	93.05	111	123.00	33

Scan 514 (13.552 min): A0331.D

Modified:subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.05	66						
125.80	64						
127.80	54						
130.00	142						
131.15	30						
131.90	81						
133.00	125						
134.00	2002						
135.00	308						
136.00	128						

Compounds from Proctor and Gamble A0331.D

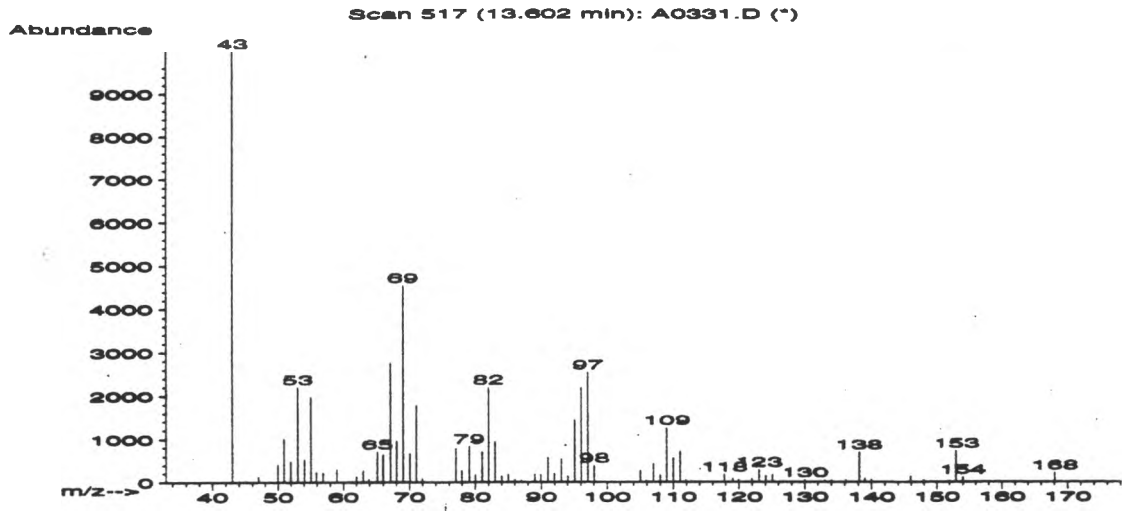
Scan 514 (13.552 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-Propanone, 1-phenyl-	134	C9H10O	90
2.	1-Propanone, 1-phenyl-	134	C9H10O	78
3.	Benzoic acid, methyl ester	136	C8H8O2	64
4.	Benzeneacetic acid, .alpha.-oxo-, ethyl	178	C10H10O3	64
5.	Benzoic acid, methyl ester	136	C8H8O2	64
6.	Benzoic acid, methyl ester	136	C8H8O2	64
7.	Benzeneacetic acid, .alpha.-oxo-, methyl	164	C9H8O3	64
8.	1,2-Propanedione, 1-phenyl-	148	C9H8O2	64
9.	Benzoyl chloride	140	C7H5ClO	64
10.	Benzoic acid, methyl ester	136	C8H8O2	64
11.	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	64
12.	PHENYL-GLYOXYLIC ACID	150	C8H6O3	59
13.	2-PHENYLOXETANE	134	C9H10O	59
14.	Ethanedione, diphenyl-	210	C14H10O2	59
15.	Benzoyl bromide	184	C7H5BrO	53
16.	Benzoic acid, methyl ester	136	C8H8O2	53
17.	Benzoyl chloride	140	C7H5ClO	53
18.	1(3H)-Isobenzofuranone	134	C8H6O2	53
19.	2-Phenyl-3-oxetanone	148	C9H8O2	53
20.	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	50

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000093-55-0	121570	67	17	0	83	5	57	6	47	9734
2.	*78	000093-55-0	7383	54	29	1	99	9	46	8	38	9898
3.	64	000093-58-3	121835	54	39	2	74	19	37	0	39	9643
4.	64	001603-79-8	24579	49	38	1	75	19	37	10	41	9821
5.	64	000093-58-3	121839	53	33	2	80	19	37	5	40	9643
6.	64	000093-58-3	121844	43	45	1	88	20	37	0	39	9482
7.	64	015206-55-0	125272	63	24	0	66	19	37	0	38	9701
8.	64	000579-07-7	11943	56	29	0	82	19	37	0	39	9824
9.	64	000098-88-4	122406	50	37	0	70	19	37	14	41	9662
10.	64	000093-58-3	121842	53	33	2	81	19	37	5	40	9582
11.	64	000936-59-4	20160	54	25	0	82	19	37	11	40	9783
12.	59	000000-00-0	12531	53	30	1	98	23	33	4	39	9801
13.	*59	004436-23-1	7408	46	64	2	73	23	33	0	40	9648
14.	59	000134-81-6	129118	55	29	0	89	21	33	2	41	9847
15.	53	000618-32-6	27174	47	49	0	74	27	28	0	39	9775
16.	53	000093-58-3	121840	57	36	1	58	27	28	0	39	9285
17.	53	000098-88-4	122405	47	40	0	74	27	28	0	39	9775
18.	*53	000087-41-2	121549	35	29	2	79	30	28	0	39	9752
19.	53	087385-78-2	11961	43	44	0	66	29	28	0	39	9738
20.	50	000936-59-4	125725	45	33	1	73	31	25	19	41	9678

Peak 41



Scan 517 (13.602 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	10000	62.00	137	77.05	788	89.00	185
46.95	138	63.00	278	77.95	277	89.90	181
49.95	416	63.90	71	79.05	832	91.00	577
50.95	1009	65.15	703	80.00	181	91.95	200
51.95	482	66.00	636	81.00	708	93.05	540
53.05	2193	67.15	2761	82.00	2197	94.05	150
54.05	534	68.05	958	83.00	939	95.05	1435
55.05	1970	69.05	4545	84.00	146	96.05	2191
55.90	238	70.05	661	85.00	188	97.05	2542
56.90	225	71.05	1782	86.00	67	98.05	389
59.00	297	71.95	92	87.00	43	103.05	21

Scan 517 (13.602 min): A0331.D

Modified:scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.00	279	119.95	60	140.00	60		
105.90	36	121.95	75	145.95	146		
107.00	433	123.05	296	147.95	51		
108.00	171	124.05	150	152.05	31		
109.00	1258	125.05	171	153.00	728		
110.00	556	130.00	52	154.00	119		
111.00	716	133.00	40	168.05	221		
111.90	51	134.00	48				
112.75	32	136.15	43				
117.80	180	138.15	700				
119.05	87	139.00	90				

Compounds from Proctor and Gamble A0331.D

Scan 517 (13.602 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Spiro[5.6]dodecane	166	C12H22	47
2.	Olealdehyde, dimethyl acetal	312	C20H40O2	42
3.	2,4-DIMETHYLCYCLOPENT-4-ENE-1,3-DIONE	124	C7H8O2	40
4.	Cyclododecene	166	C12H22	38
5.	2-Nonenal, 8-oxo-	154	C9H14O2	35
6.	2,4-Hexadienal	96	C6H8O	35
7.	2,3-Hexadiene, 2-methyl-	96	C7H12	35
8.	Citronellyl acetate	198	C12H22O2	35
9.	Undecanenitrile	167	C11H21N	32
10.	3-Heptyn-2-ol	112	C7H12O	32
11.	5-Dodecen-1-ol, acetate, (Z)-	226	C14H26O2	32
12.	3-Octyne	110	C8H14	30
13.	2-Butenal, 2-ethenyl-	96	C6H8O	27
14.	E6-DODECENYLACETATE	226	C14H26O2	25
15.	(E)-1-(1-Butenyl)aziridine	97	C6H11N	22
16.	2-Hexyne, 5-methyl-	96	C7H12	22
17.	1,3,3-TRIMETHYL-2-OXABICYCLO[2.2.2]OCTAN	168	C10H16O2	14
18.	2,5-OCTADIENE	110	C8H14	14
19.	ISO-MENTHYL ACETATE	198	C12H22O2	12
20.	Cyclohexanol, 5-methyl-2-(1-methylethyl)	198	C12H22O2	12

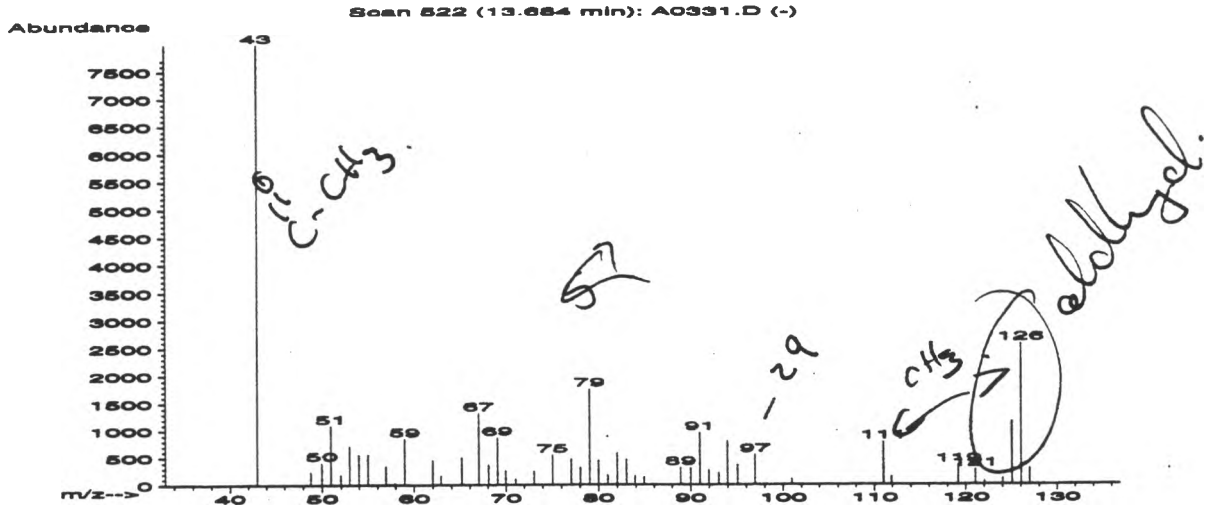
	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	47	000181-15-7	125612	54	36	0	22	40	20	0	39	8634
2.	42	015677-71-1	77791	53	95	2	84	29	17	0	36	8894
3.	40	000000-00-0	4691	43	67	2	70	33	16	0	37	8462
4.	38	001501-82-2	125606	44	58	0	28	48	14	0	39	8093
5.	35	077611-52-0	14377	45	57	2	92	55	11	18	38	7774
6.*	35	000142-83-6	575	41	61	0	25	53	11	0	39	7569
7.*	35	029212-09-7	622	44	52	1	29	51	11	0	40	7389
8.	35	000150-84-5	33918	56	45	2	89	55	11	13	38	6944
9.	32	002244-07-7	125667	44	52	1	20	48	9	0	37	7111
10.	32	056699-62-8	2577	43	56	2	39	48	9	0	35	7838
11.	32	016676-96-3	46799	53	61	2	37	46	9	0	36	8035
12.*	30	015232-76-5	2218	55	40	2	45	59	9	0	49	7123
13.*	27	020521-42-0	576	40	25	0	21	57	8	19	38	7460
14.	25	000000-00-0	46801	45	73	3	75	53	7	10	37	7706
15.*	22	080839-92-5	692	34	49	0	34	64	5	0	41	6722
16.*	22	053566-37-3	606	33	70	0	25	62	5	0	41	6217
17.*	14	101221-23-2	20521	33	43	0	75	70	2	10	39	5877
18.*	14	000000-00-0	2226	44	54	1	32	66	2	0	39	6389
19.	12	020777-45-1	33966	47	81	2	85	61	2	0	35	4530
20.	12	016409-45-3	33959	47	81	2	80	61	2	0	35	4495

Coeluting
168
+ 138.

goes 168 - 15
↓
153

$C_{10}H_{16}O_2$

Peak 42



Scan 522 (13.684 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	7995	62.00	449	78.05	317	91.95	269
48.80	250	62.90	164	79.05	1758	93.05	216
49.95	407	65.15	501	80.00	440	93.95	805
50.95	1088	67.00	1315	81.00	181	95.05	369
51.95	183	68.05	365	82.00	585	96.95	549
52.95	716	69.05	863	83.00	463	100.95	99
53.95	550	69.95	262	83.90	163	110.10	7
54.95	556	71.05	108	84.90	140	111.00	785
56.90	340	73.05	251	88.90	314	111.90	148
57.90	30	75.05	547	90.00	307	119.20	351
59.00	846	77.05	472	91.00	959	121.05	278

Scan 522 (13.684 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.05	63						
124.05	105						
125.05	1162						
126.05	2576						
126.95	295						

Compounds from Proctor and Gamble A0331.D

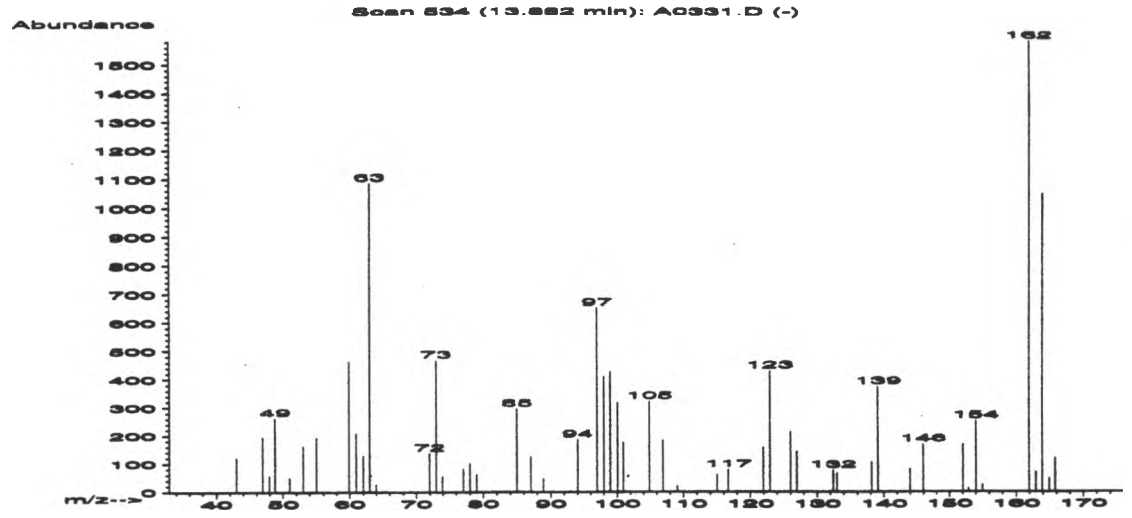
Scan 522 (13.684 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2,2-DIMETHYL-4,5-DIMETHYLEN-1,3-DIOXOLAN	126	C7H10O2	25
2.	6-Nonynoic acid	154	C9H14O2	14
3.	2,4(1H,3H)-Pyrimidinedione, 6-methyl-	126	C5H6N2O2	10
4.	1-Azabicyclo[2.2.2]octane, 4-methyl-	125	C8H15N	10
5.	1-Azabicyclo[2.2.2]octane, 4-methyl-	125	C8H15N	10
6.	3-Azabicyclo[3.2.2]nonane	125	C8H15N	10
7.	1-Cyclohexene-1-methanol	112	C7H12O	10
8.	3-HEXEN-2-ONE, 3,4-DIMETHYL-, CIS/TRANS	126	C8H14O	9
9.	3-Hexen-2-one, 3,4-dimethyl-	126	C8H14O	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*25	070517-23-6	5198	32	19	0	30	55	7	0	33	7655
2.	14	056630-31-0	14374	45	41	0	23	70	2	0	39	5222
3.	*10	000626-48-2	5101	33	58	3	85	80	1	0	39	6950
4.	*10	045651-41-0	120463	34	47	1	27	80	1	0	39	4624
5.	*10	045651-41-0	5040	35	51	1	32	80	1	0	39	4185
6.	*10	000283-24-9	5044	33	57	0	19	77	1	0	41	3823
7.	*10	004845-04-9	2635	34	35	0	15	72	1	19	39	5316
8.	* 9	020685-46-5	5315	40	52	2	67	75	1	0	35	6717
9.	* 9	001635-02-5	120591	40	52	2	67	75	1	0	35	6717

Peak 44



Scan 534 (13.882 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	121	63.95	27	96.95	649	122.95	429
46.95	195	71.95	137	98.00	409	126.00	214
47.95	57	72.95	466	98.95	427	126.95	143
48.80	262	73.90	54	100.05	315	132.40	77
51.00	50	77.05	81	100.95	176	133.00	65
53.00	162	78.00	101	104.90	321	138.15	106
55.00	193	79.05	61	106.95	184	139.15	373
59.90	462	85.00	295	109.05	21	143.95	81
60.95	207	87.00	124	115.00	61	145.95	169
62.00	128	88.90	47	116.70	79	152.05	168
63.00	1083	94.00	186	121.95	158	152.90	13

Scan 534 (13.882 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
154.00	252						
155.00	26						
161.90	1583						
162.90	69						
163.90	1048						
164.90	47						
165.80	119						

Compounds from Proctor and Gamble A0331.D

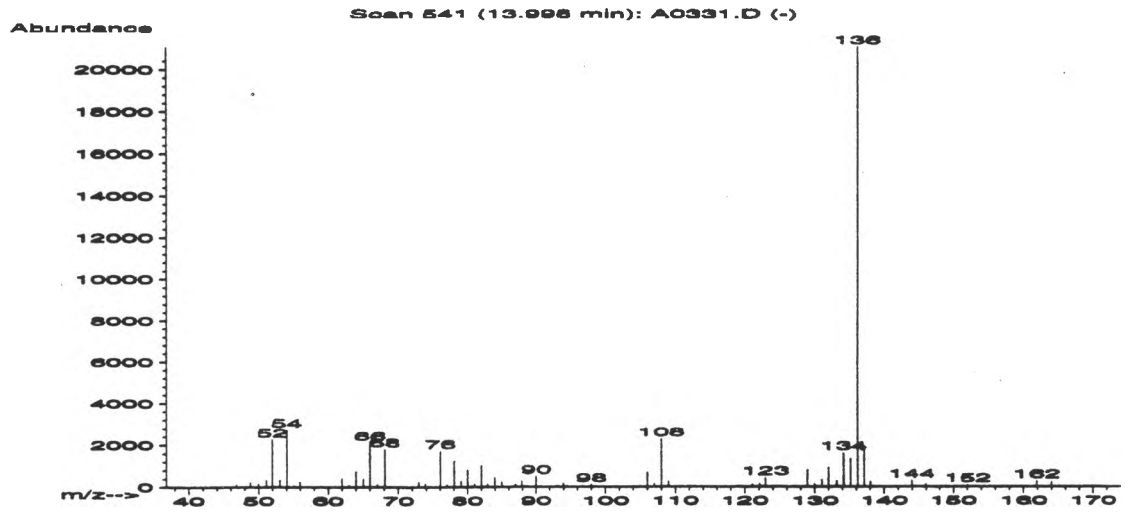
Scan 534 (13.882 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2,3-dichloro-	162	C6H4Cl2O	76
2.	Phenol, 2,5-dichloro-	162	C6H4Cl2O	68
3.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	58
4.	Phenol, 2,3-dichloro-	162	C6H4Cl2O	53
5.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	53
6.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	53
7.	Phenol, 2,6-dichloro-	162	C6H4Cl2O	53
8.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	53
9.	Phenol, 2,3-dichloro-	162	C6H4Cl2O	42
10.	Phenol, 2,6-dichloro-	162	C6H4Cl2O	42
11.	Phenol, 3,5-dichloro-	162	C6H4Cl2O	40
12.	Phenol, 2,6-dichloro-	162	C6H4Cl2O	37
13.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	27
14.	Butane, 1,1'-sulfinylbis-	162	C8H18OS	25
15.	1H-Benzotriazole, 5-nitro-	164	C6H4N4O2	23
16.	Phenol, 3,4-dichloro-	162	C6H4Cl2O	22
17.	Phenol, 2,6-dichloro-	162	C6H4Cl2O	16
18.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	16
19.	2-Pyridinamine, 3,5-dichloro-	162	C5H4Cl2N2	12
20.	Phenol, 2,4-dichloro-	162	C6H4Cl2O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*76	000576-24-9	125027	68	66	2	68	23	45	0	68	9201
2.	*68	000583-78-8	125036	68	56	1	71	23	40	0	53	9302
3.	*58	000120-83-2	125030	62	71	1	74	27	32	0	46	9119
4.	*53	000576-24-9	17395	36	89	3	99	29	28	0	39	9272
5.	*53	000120-83-2	125035	65	52	1	68	26	28	10	40	8805
6.	*53	000120-83-2	125029	44	79	2	93	29	28	5	38	9208
7.	*53	000087-65-0	125041	67	51	1	79	30	28	0	39	9002
8.	*53	000120-83-2	125031	44	78	2	91	27	28	0	40	9243
9.	*42	000576-24-9	125026	36	86	2	99	29	17	12	37	9271
10.	*42	000087-65-0	125039	54	69	1	68	26	17	0	35	9254
11.	*40	000591-35-5	125045	52	60	1	68	34	16	1	31	8297
12.	37	000087-65-0	17398	50	68	0	55	44	13	6	31	8819
13.	*27	000120-83-2	17396	48	61	1	94	60	8	0	39	8879
14.	*25	002168-93-6	125079	29	93	3	235	45	7	0	29	7709
15.	*23	002338-12-7	18183	28	99	1	66	50	6	2	28	6301
16.	*22	000095-77-2	125044	52	52	2	99	63	5	0	39	8396
17.	*16	000087-65-0	125040	34	74	2	99	60	3	0	30	8888
18.	*16	000120-83-2	125033	59	71	2	99	59	3	0	37	9085
19.	*12	004214-74-8	17379	33	88	2	99	65	2	0	30	7888
20.	10	000120-83-2	125032	40	72	0	60	69	1	0	33	9141

Peak 45



Scan 541 (13.998 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
46.80	115	62.00	427	78.05	1227	92.85	20
48.80	227	63.00	65	79.05	277	93.95	166
49.95	169	64.00	748	80.00	813	98.00	120
51.05	326	65.00	400	81.00	129	104.95	51
51.95	2264	66.00	2110	82.00	994	106.00	698
53.00	341	67.00	118	82.95	131	107.00	152
54.05	2735	68.05	1801	83.95	449	108.00	2303
55.00	64	72.95	234	85.00	260	109.05	265
55.95	259	73.90	162	87.00	127	112.00	29
58.95	56	76.05	1710	87.90	305	121.05	116
61.00	45	77.05	92	90.00	499	122.05	136

Scan 541 (13.998 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.95	445	143.95	297				
128.90	793	145.95	126				
130.00	129	152.05	98				
131.00	344	161.90	288				
132.00	921	164.00	245				
133.15	282						
134.15	1631						
135.15	1335						
136.15	21066						
137.15	1925						
138.05	256						

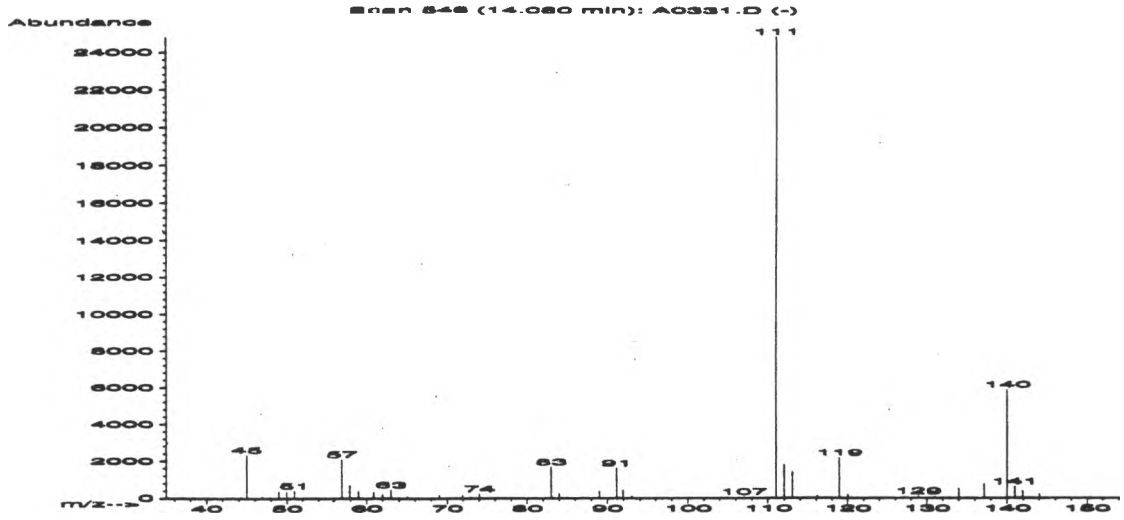
Scan 541 (13.998 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Naphthalene-d8	128	C10D8	81
2.	6H-Purin-6-one, 1,7-dihydro-	136	C5H4N4O	59
3.	2,1,3-Benzothiadiazole	136	C6H4N2S	53
4.	Pyrazine, 2,3-dimethyl-5-(1-methylpropyl	164	C10H16N2	50
5.	Benzaldehyde, 4-methoxy-	136	C8H8O2	50
6.	Inosine	268	C10H12N4O5	45
7.	Benzamide, 3-amino-	136	C7H8N2O	42
8.	6H-Purin-6-one, 1,7-dihydro-	136	C5H4N4O	42
9.	2-HYDROXY-3-METHYLBENZALDEHYDE	136	C8H8O2	38
10.	Benzaldehyde, 3-methoxy-	136	C8H8O2	38
11.	6H-Purin-6-one, 1,7-dihydro-	136	C5H4N4O	38
12.	3-DEUTERIO-1,2-BENZISOTHIAZOLE	135	C7H4DNS	36
13.	Pyrrolidine, 1-(1-cyclopenten-1-yl)-	137	C9H15N	36
14.	2,1,3-Benzothiadiazole	136	C6H4N2S	36
15.	Pyrrolidine, 1-(1-cyclopenten-1-yl)-	137	C9H15N	36
16.	Pyrazine, tetramethyl-	136	C8H12N2	36
17.	2H-Quinolizine, 1,3,4,6,7,9a-hexahydro-	137	C9H15N	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*81	000000-00-0	6077	66	25	1	66	16	49	0	64	9921
2.	*59	000068-94-0	121783	34	51	3	98	23	33	0	39	9881
3.	*53	000273-13-2	7732	37	52	3	82	28	28	0	39	9836
4.	50	032263-00-6	125348	40	56	1	80	17	25	10	31	8666
5.	*50	000123-11-5	121857	33	77	3	82	32	25	0	39	9809
6.	45	000058-63-9	62487	43	91	3	83	21	19	0	35	9916
7.	*42	003544-24-9	7777	29	57	3	89	28	17	1	30	9845
8.	*42	000068-94-0	121781	36	39	2	94	26	17	3	32	9845
9.	*38	000824-42-0	7825	29	89	1	89	25	14	0	29	7513
10.	*38	000591-31-1	121853	28	95	2	83	25	14	0	29	7905
11.	*38	000068-94-0	121782	29	51	2	99	23	14	0	29	9863
12.	*36	040991-32-0	7532	32	56	3	95	30	12	0	27	9823
13.	36	007148-07-4	122161	34	65	2	90	28	12	0	22	9393
14.	*36	000273-13-2	121802	32	68	2	79	28	12	0	29	9840
15.	36	007148-07-4	8325	35	67	2	99	28	12	0	20	9532
16.	*36	001124-11-4	121881	34	68	1	92	26	12	0	25	9834
17.	28	001004-90-6	8334	34	75	2	85	37	8	0	21	8398

Peak 46



Scan 546 (14.080 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.95	2342	65.00	76	93.00	102	131.00	68
46.85	72	69.00	167	104.95	21	134.00	519
48.95	338	71.95	153	107.00	64	137.15	760
49.95	314	72.95	47	111.00	24777	140.00	5828
50.95	398	74.05	235	112.00	1778	140.95	618
56.90	2101	83.00	1683	113.00	1370	141.95	363
57.90	690	84.00	231	115.00	23	144.05	214
59.00	359	86.95	47	116.15	114		
60.90	312	89.00	401	118.95	2173		
62.00	194	91.15	1610	120.05	173		
63.00	445	91.95	435	128.90	90		

Compounds from Proctor and Gamble A0331.D

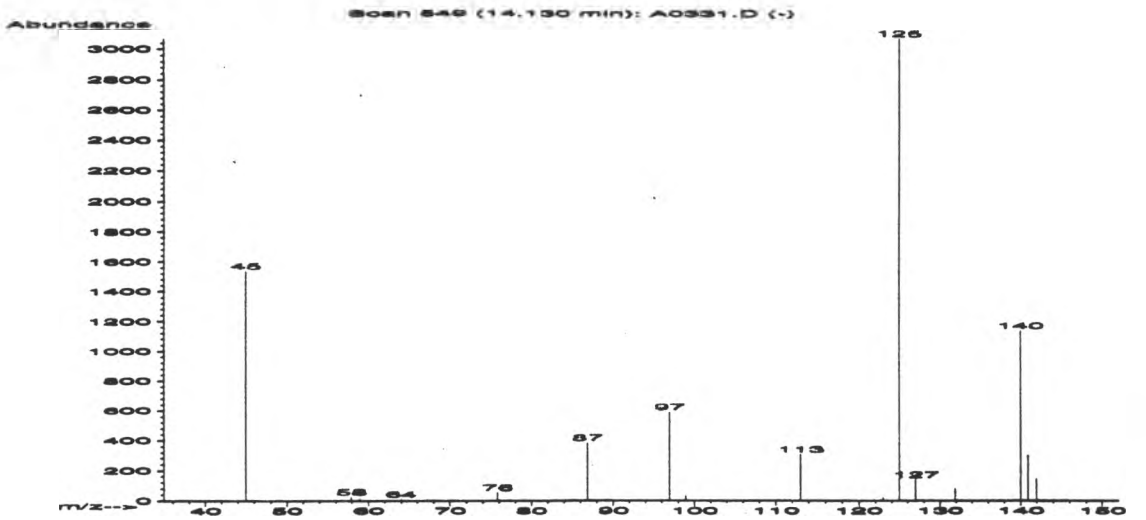
Scan 546 (14.080 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-(2-THIENYL)PROPANAL	140	C7H8OS	78
2.	Thiophene, 2-methyl-5-propyl-	140	C8H12S	78
3.	Thiophene, 2-methyl-5-propyl-	140	C8H12S	72
4.	2H-Pyran-2-carboxaldehyde, 3,4-dihydro-2	140	C8H12O2	50
5.	2H-Pyran-2-carboxaldehyde, 3,4-dihydro-2	140	C8H12O2	50
6.	4-MERCAPTOPYRIDINE	111	C5H5NS	33
7.	2-PROPIONYLTHIOPHENE	140	C7H8OS	22
8.	METHYL 3-THIOPHENECARBOXYLATE	142	C6H6O2S	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	063362-05-0	9081	39	3	0	99	6	46	3	42	9910
2.	*78	033933-73-2	122461	44	41	1	84	7	46	0	40	9944
3.	*72	033933-73-2	9277	44	36	0	93	14	42	5	40	9910
4.	*50	001920-21-4	122450	28	42	0	78	20	25	0	33	9886
5.	*50	001920-21-4	9217	28	57	1	79	20	25	0	33	9900
6.	*33	004556-23-4	2328	31	65	1	71	33	10	0	29	9647
7.	*22	000000-00-0	9086	34	38	0	17	64	5	0	41	8673
8.	*10	000000-00-0	9797	25	43	0	63	61	1	1	26	9444

Peak 47



Scan 549 (14.130 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.95	1536	127.00	136				
57.90	23	131.90	77				
58.95	11	140.00	1142				
63.95	8	140.90	301				
75.80	51	141.95	144				
86.90	384						
96.95	589						
98.95	35						
113.00	306						
122.95	20						
124.95	3067						

Compounds from Proctor and Gamble A0331.D

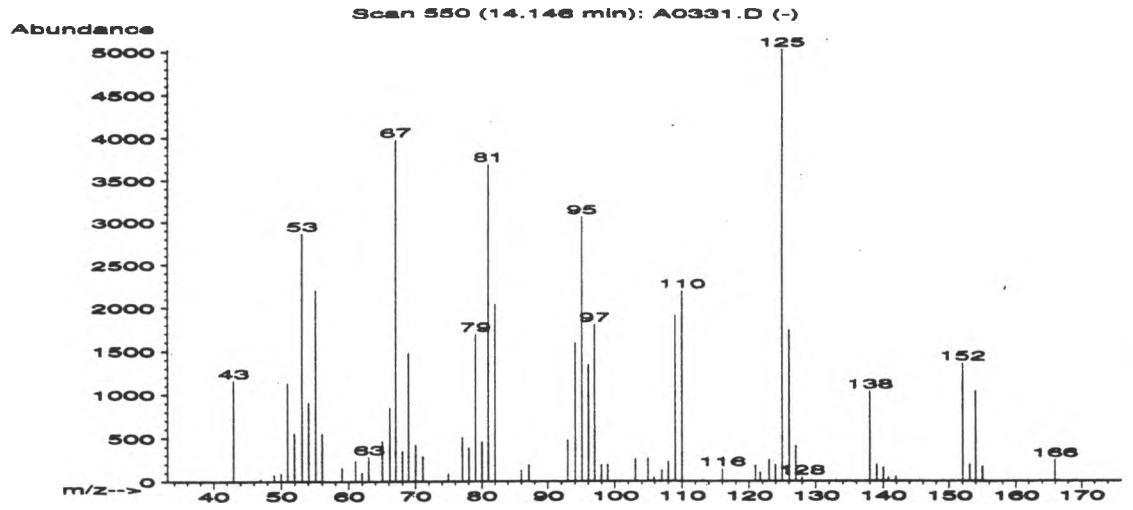
Scan 549 (14.130 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Thiophene, 2-(1,1-dimethylethyl)-	140	C8H12S	59
2.	2-ACETYL-3-METHYLTHIOPHENE	140	C7H8OS	53
3.	Thiophene, 3-(1,1-dimethylethyl)-	140	C8H12S	42

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	001689-78-7	9275	31	65	0	89	22	33	9	42	9390
2.	*53	000000-00-0	9087	33	62	0	77	30	28	0	41	9453
3.	*42	001689-79-8	9276	29	67	0	99	27	17	2	35	9454

Peak 48
Coeluting Monoterpenes



Scan 550 (14.146 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1157	61.00	237	77.05	509	95.05	3067
46.95	32	61.95	101	78.05	387	96.05	1341
48.95	74	63.00	283	79.05	1691	96.95	1805
49.95	96	65.00	463	80.00	454	97.95	188
50.95	1132	66.15	848	81.00	3671	98.95	191
51.95	562	67.00	3960	82.00	2038	103.05	260
53.05	2867	68.00	349	83.95	4	105.00	265
54.05	911	68.95	1474	86.00	127	105.90	42
55.05	2205	70.00	421	87.15	193	107.00	128
56.00	550	71.05	290	92.95	483	108.00	226
58.95	160	74.95	89	94.05	1597	109.00	1916

Scan 550 (14.146 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
110.00	2195	138.00	1038				
116.00	143	139.05	198				
120.95	181	140.00	159				
121.70	101	140.80	41				
123.00	247	141.90	57				
123.95	187	152.05	1365				
124.95	5027	153.15	196				
126.05	1746	154.00	1039				
127.05	409	155.00	169				
127.95	46	165.95	247				
133.00	14						

Compounds from Proctor and Gamble A0331.D

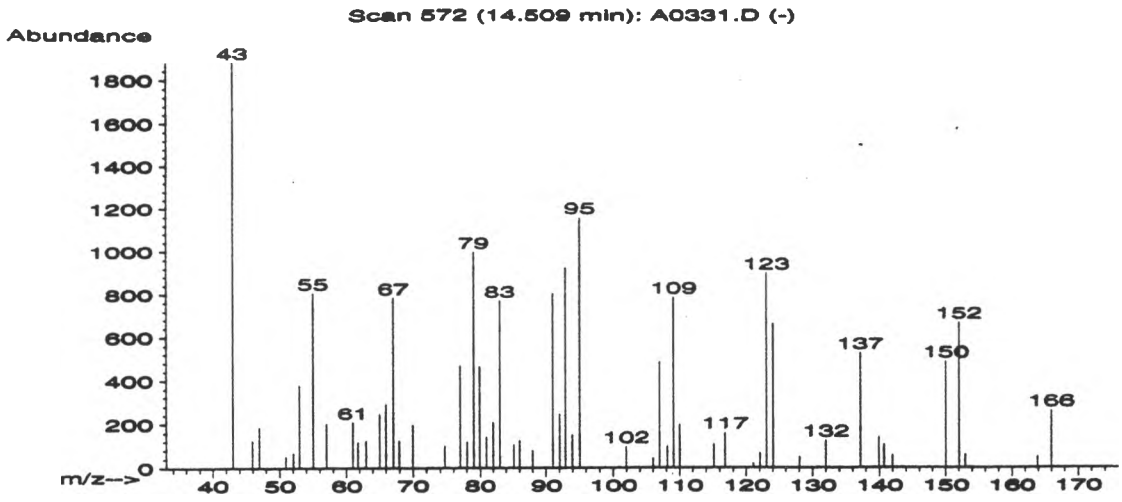
Scan 550 (14.146 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclohexane, 1-methyl-4-(1-methylethylid	138	C10H18	46
2.	3-ETHYLCYCLOPENT-2-EN-1-ONE	110	C7H10O	38
3.	Bicyclo[4.1.0]heptan-2-one, 3,5,5-trimet	152	C10H16O	38
4.	2,4-Heptadienal, (E,E)-	110	C7H10O	38
5.	1-(ETHYL-1-D)-2-PYRIDONE	123	C7H7D2NO	38
6.	13	154	C9H14S	30
7.	4-Octyne	110	C8H14	30
8.	Cyclohexanone, 2-methyl-5-(1-methylethen	152	C10H16O	25
9.	Dihydrocarvone	152	C10H16O	25
10.	Naphthalene, decahydro-2-methyl-	152	C11H20	20
11.	2-METHYLDECALIN (PROBABLY TRANS)	152	C11H20	20
12.	3-Octyne	110	C8H14	18
13.	(-)-TRANS-CARANON-(3)	152	C10H16O	18
14.	(-)-TRANS-CARANON-(3)	152	C10H16O	15
15.	CYCLOPENTANE, 1-METHYL-3-(2-METHYLPROPEN	138	C10H18	15
16.	TRANS-DIMETHYL-ISOPROPYLIDENE CYCLOPROPA	110	C8H14	11
17.	CIS-SYN-2-METHYL-DECAHYDRONAPHTHALENE	152	C11H20	11
18.	3-Octyne, 5-methyl-	124	C9H16	11
19.	Naphthalene, decahydro-2-methyl-	152	C11H20	11
20.	2-METHYL-2,3-DIVINYLOXIRAN	110	C7H10O	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	001124-27-2	122318	64	52	2	75	41	20	18	47	6290
2.	*38	000000-00-0	2186	36	63	0	72	51	14	4	43	6255
3.	*38	029750-24-1	13725	73	54	2	61	61	14	42	68	6318
4.	*38	004313-03-5	2160	48	70	2	98	54	14	0	44	6377
5.	*38	053907-48-5	4558	59	51	2	96	60	14	0	51	8342
6.	*30	060813-89-0	14512	43	23	0	87	56	9	18	47	6112
7.	*30	001942-45-6	118881	53	59	2	97	59	9	0	47	6403
8.	*25	007764-50-3	13846	49	76	2	78	65	7	0	46	7140
9.	*25	005948-04-9	123991	49	76	2	78	65	7	0	46	7140
10.	*20	002958-76-1	124047	68	56	1	72	67	4	31	58	6543
11.	*20	002958-76-1	13881	68	56	1	72	67	4	31	58	6543
12.	*18	015232-76-5	118879	63	46	1	72	67	3	10	47	6716
13.	*18	004176-04-9	124001	65	25	0	67	69	3	20	47	6174
14.	*15	004176-04-9	13728	69	48	0	67	73	2	24	58	6180
15.	*15	000000-00-0	8777	62	52	1	72	71	2	0	51	6112
16.	*11	000000-00-0	2262	50	57	1	59	72	2	0	46	6212
17.	*11	000000-00-0	13879	49	59	1	46	80	2	0	44	6243
18.	*11	062108-33-2	4874	51	64	0	67	72	2	0	46	6752
19.	*11	002958-76-1	124049	49	59	1	46	80	2	0	44	6243
20.	*11	070597-13-6	2175	34	41	0	72	73	2	4	43	6153

Peak 49
Coeluting Compounds



Scan 572 (14.509 min): A0331.D

Modified:subtracted

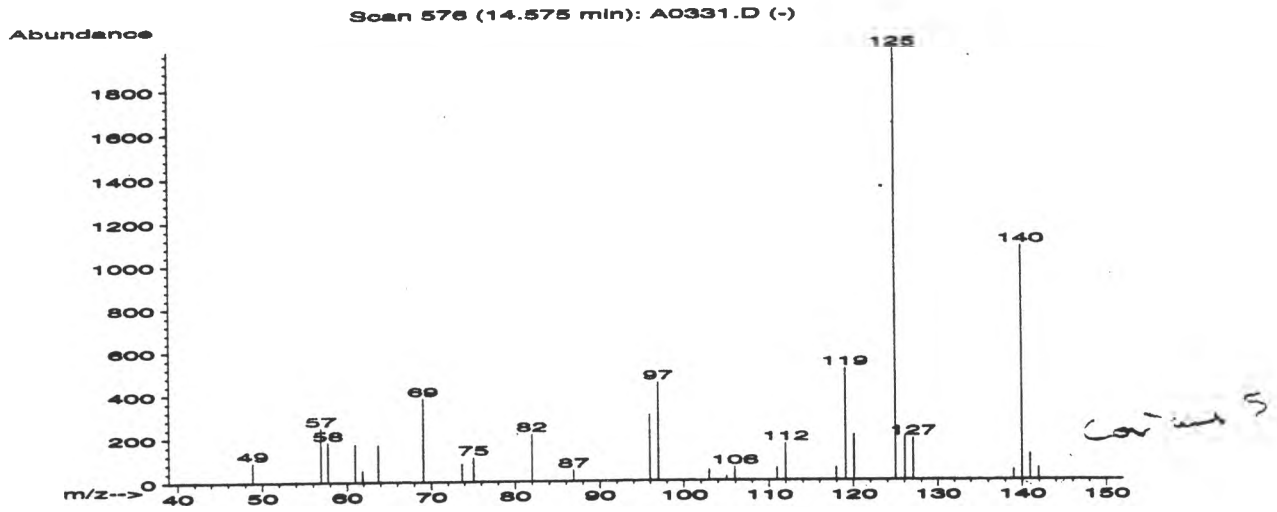
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1880	65.00	248	82.00	207	106.00	42
45.95	125	66.00	292	83.00	770	106.95	487
46.95	184	67.10	783	85.15	106	108.15	98
50.95	51	67.95	125	86.00	127	109.10	786
52.05	67	69.95	196	88.00	78	110.00	196
52.95	379	74.70	101	91.05	805	115.15	108
55.00	806	77.00	470	92.05	246	116.80	160
57.00	201	78.05	121	92.95	924	121.05	21
61.00	209	79.05	995	93.95	152	122.05	67
61.75	118	79.90	465	95.05	1156	123.05	899
63.00	124	80.95	143	101.95	96	124.05	661

Scan 572 (14.509 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
128.05	49						
132.00	125						
137.15	526						
139.90	140						
140.70	107						
141.95	55						
150.05	487						
152.05	667						
153.00	61						
163.90	51						
165.95	261						

Peak 50



Scan 576 (14.575 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.90	91	86.90	49	124.95	1983		
53.95	5	95.95	301	126.05	198		
56.95	246	97.00	452	127.05	190		
57.75	179	102.95	47	139.00	45		
60.95	172	105.00	18	140.00	1080		
61.85	52	105.95	59	140.95	117		
63.75	169	110.95	56	141.95	54		
69.05	382	112.00	168				
73.70	82	117.95	57				
75.05	110	119.05	514				
82.00	215	120.05	206				

Compounds from Proctor and Gamble A0331.D

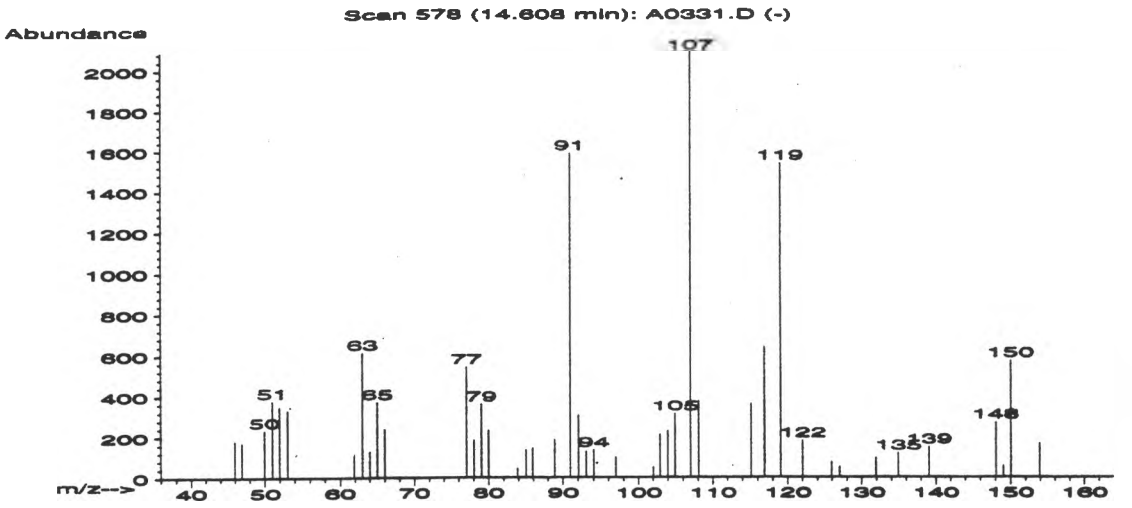
Scan 576 (14.575 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 4-(methylthio)-	140	C7H8OS	64
2.	Cyclohexanone, 2-acetyl-	140	C8H12O2	53
3.	Benzene, 1-chloro-4-ethyl-	140	C8H9Cl	50
4.	Benzene, 1-chloro-2-ethyl-	140	C8H9Cl	50
5.	1-METHOXY-6,6-DIMETHYLCYCLOHEXENE	140	C9H16O	50
6.	2-Cyclopentene-1-thione, 3,4,4-trimethyl	140	C8H12S	50
7.	Benzene, (methylsulfinyl)-	140	C7H8OS	46
8.	2-ACETYL-3-METHYLTHIOPHENE	140	C7H8OS	42
9.	METHYLESTER OF 2-METHYLENE-3-HEXENE CARB	140	C8H12O2	40
10.	(+,-)-2,3,3-Trimethyl-4-hydroxymethylcyc	140	C9H16O	40
11.	Benzenethiol, 2-amino-	125	C6H7NS	38
12.	2(1H)-Pyridinethione, 5-methyl-	125	C6H7NS	37
13.	Benzenethiol, 2-amino-	125	C6H7NS	37
14.	2(1H)-Pyridinone, 4-hydroxy-6-methyl-	125	C6H7NO2	37
15.	2-AMINO-6-METHYL-4-PYRIMIDINOL	125	C5H7N3O	37
16.	2-Butanone, (1-methyl-2-propenyl)hydrazo	140	C8H16N2	33
17.	2-Butenal, diethylhydrazone	140	C8H16N2	32
18.	1,2-Benzenediol, 3-methoxy-	140	C7H8O3	27
19.	3-Methoxy-pyrocatechol	140	C7H8O3	27
20.	Phenol, 2-(methylthio)-	140	C7H8OS	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	001073-72-9	122414	48	48	2	98	24	37	3	47	8882
2.	*53	000874-23-7	9238	48	46	0	69	26	28	15	41	9510
3.	*50	000622-98-0	9148	35	52	2	79	35	25	11	40	9152
4.	*50	000089-96-3	9146	35	69	2	99	35	25	0	39	9205
5.	*50	073741-66-9	9396	43	43	1	93	34	25	12	38	9514
6.	*50	030221-53-5	9281	35	66	0	93	35	25	0	41	9421
7.	*46	001193-82-4	9090	37	63	0	59	45	20	2	43	9123
8.	*42	000000-00-0	9087	41	55	1	99	26	17	0	35	9567
9.	*40	072707-70-1	9173	30	30	0	86	34	16	0	33	9409
10.	*40	000000-00-0	9372	32	66	0	99	35	16	0	33	9426
11.	*38	000137-07-5	120453	28	83	0	99	40	14	0	33	8550
12.	*37	018368-58-6	4970	31	81	0	99	42	13	0	33	8513
13.	*37	000137-07-5	120454	28	60	0	99	42	13	0	33	8504
14.	*37	003749-51-7	120451	31	66	0	84	41	13	0	33	8573
15.	*37	000000-00-0	4946	31	75	0	94	42	13	0	33	8569
16.	*33	036566-77-5	9286	31	84	1	112	35	10	0	29	9425
17.	*32	025186-07-6	9284	35	59	1	61	50	9	3	32	9205
18.	*27	000934-00-9	9119	35	63	0	52	57	8	0	41	8655
19.	*27	000000-00-0	9121	35	63	0	52	57	8	0	41	8655
20.	*25	001073-29-6	122413	30	66	0	52	55	7	0	33	7488

Peak 51



Scan 578 (14.608 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
45.95	179	77.05	546	94.05	136	122.05	182
46.90	171	78.05	185	96.95	100	125.95	76
49.95	234	79.05	362	102.05	51	127.00	50
51.00	377	80.00	233	102.95	212	131.90	93
51.95	348	83.90	45	104.00	229	134.90	120
53.05	331	85.00	135	104.95	314	139.05	150
61.90	107	85.90	146	107.00	2088	148.05	271
63.00	613	88.90	187	108.10	375	149.05	57
64.00	128	91.00	1589	115.15	362	150.05	576
65.00	372	92.05	307	116.95	642	153.90	168
66.00	239	93.05	130	119.05	1540		

Scan 578 (14.608 min): A0331.D

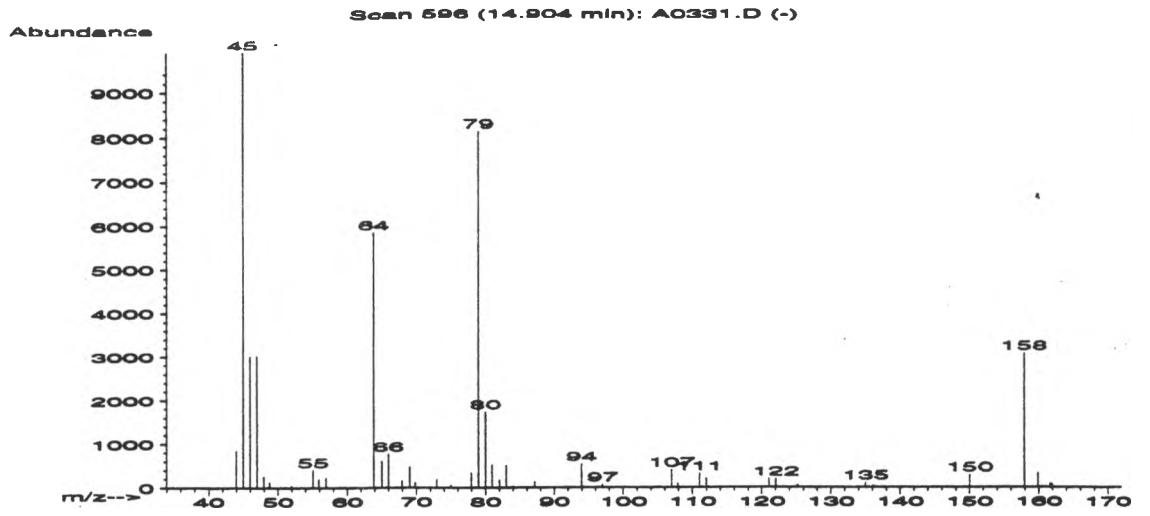
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Pyridine, 2,4-dimethyl-	107	C7H9N	38
2.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	38
3.	Aziridine, 1-phenyl-	119	C8H9N	38
4.	3,7,7-TRIMETHYL-CYCLOHEPTA-1,3,5-TRIENE	134	C10H14	38
5.	Benzeneethanol, ar-ethyl-	150	C10H14O	38
6.	Phenol, 2-(2-methylpropyl)-	150	C10H14O	35
7.	2-Pyridinemethanamine, .alpha.-methyl-	122	C7H10N2	30
8.	2,5-Cyclohexadien-1-one, 4-ethyl-3,4-dim	150	C10H14O	27
9.	Phenol, 2-butyl-	150	C10H14O	27
10.	Pyridine, 3-ethyl-	107	C7H9N	25
11.	Pyridine, 3-(2-pyrrolidinyl)-, (S)-	148	C9H12N2	25
12.	Benzamide, 4-methyl-	135	C8H9NO	25
13.	Pyridine, 2,4-dimethyl-	107	C7H9N	25
14.	Pyridine, 3,4-dimethyl-	107	C7H9N	25
15.	Pyridine, 3-(2-pyrrolidinyl)-, (S)-	148	C9H12N2	25
16.	Pyridine, 5-ethenyl-2-methyl-	119	C8H9N	25
17.	Pyridine, 2,4-dimethyl-	107	C7H9N	22
18.	Pyridine, 2,4-dimethyl-	107	C7H9N	22
19.	Benzoyl chloride, 3-methyl-	154	C8H7ClO	22
20.	Pyridine, 2,5-dimethyl-	107	C7H9N	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	000108-47-4	118615	71	35	0	68	64	14	33	66	6619
2.	38	000099-87-6	7447	73	28	0	61	48	14	9	41	6642
3.	*38	000696-18-4	3979	58	42	0	67	55	14	7	47	6440
4.	38	000000-00-0	7465	49	40	0	76	50	14	3	38	6763
5.	*38	041673-72-7	12739	39	64	0	68	48	14	0	39	6833
6.	*35	004167-75-3	12723	37	52	0	81	55	11	0	41	7158
7.	*30	042088-91-5	4366	61	46	2	88	64	9	0	51	6575
8.	*27	017429-35-5	12775	46	64	2	69	57	8	0	40	8245
9.	*27	003180-09-4	12718	37	50	0	99	56	8	0	41	7042
10.	*25	000536-78-7	118606	49	57	1	78	64	7	0	46	6611
11.	*25	000494-97-3	123387	44	65	0	52	64	7	0	44	4960
12.	*25	000619-55-6	7559	37	54	0	63	61	7	18	43	6771
13.	*25	000108-47-4	118614	50	48	0	80	64	7	0	46	6618
14.	*25	000583-58-4	1823	48	58	1	68	64	7	0	46	6598
15.	*25	000494-97-3	11987	44	68	0	51	64	7	0	44	4950
16.	*25	000140-76-1	3976	48	53	0	73	62	7	0	46	5015
17.	*22	000108-47-4	1820	45	67	1	66	64	5	0	40	6596
18.	*22	000108-47-4	118613	46	62	2	99	65	5	0	40	6615
19.	*22	001711-06-4	14273	33	58	0	73	64	5	0	41	6632
20.	*22	000589-93-5	1821	44	64	1	99	64	5	0	40	6612

Peak 52

Dimethyl-tetrasulphide



Scan 596 (14.904 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	854	63.90	5838	80.95	525	121.05	200
44.95	9887	65.05	604	82.00	176	122.05	200
45.95	3012	66.00	770	83.00	508	125.15	61
46.95	3015	67.95	153	84.00	30	135.00	107
47.95	259	69.05	478	87.15	133	136.15	46
48.80	116	69.80	113	93.95	539	150.05	291
51.95	49	72.95	181	97.00	76	157.90	3058
55.05	412	75.00	62	107.00	403	159.90	322
55.90	194	77.95	339	107.90	92	161.65	87
56.90	239	78.95	8088	111.00	314	161.90	77
58.95	14	80.00	1740	112.00	206		

Compounds from Proctor and Gamble A0331.D

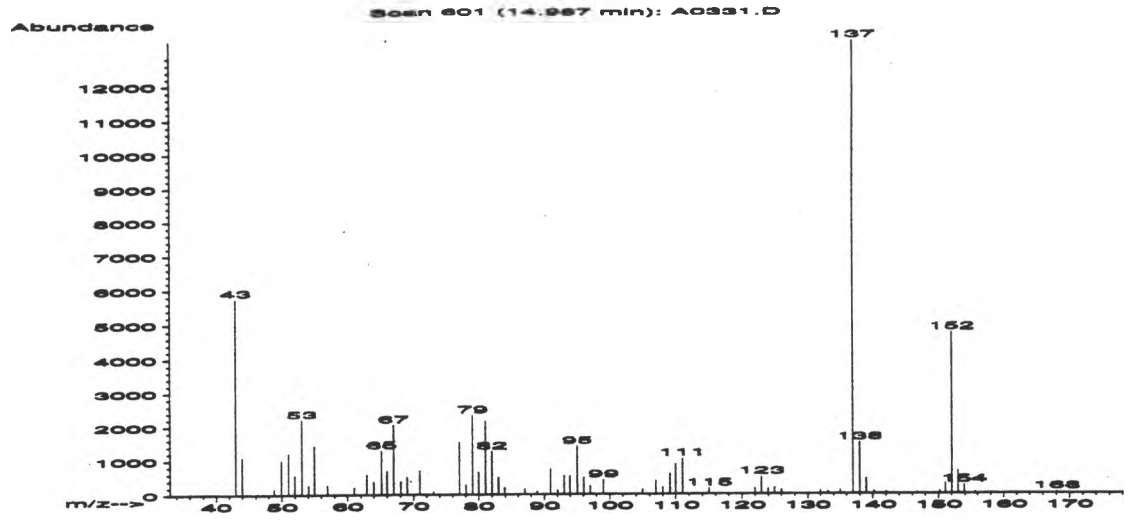
Scan 596 (14.904 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2,2'-dithiobis-	154	C4H10O2S2	36
2.	Disulfide, dimethyl	94	C2H6S2	35
3.	1,2-Ethanediol, dimethanesulfonate	218	C4H10O6S2	10
4.	3-Methylene-1,6-hexadiene	108	C8H12	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	36	001892-29-1	14171	38	95	3	117	30	12	0	28	9468
2.	*35	000624-92-0	117490	40	69	2	64	53	11	18	38	8701
3.	10	004672-49-5	42473	51	63	2	73	70	1	0	31	6359
4.	7	016626-48-5	1950	34	75	2	65	75	1	0	22	5485

Peak 53



Scan 601 (14.987 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	5752	62.90	573	79.05	2342	93.95	533
43.95	1086	64.00	390	80.00	648	95.05	1406
48.80	175	65.15	1292	81.00	2161	96.05	495
49.95	1025	66.00	688	82.00	1264	97.05	247
51.05	1215	67.00	2044	83.00	497	99.05	412
51.95	569	68.05	387	83.90	197	105.00	143
53.05	2203	69.05	506	87.00	157	107.00	397
54.05	271	70.95	692	88.90	97	108.00	198
54.95	1432	73.05	91	91.00	738	109.15	597
56.90	269	77.05	1532	92.05	130	110.00	876
61.00	213	78.05	280	93.05	527	111.00	1042

Scan 601 (14.987 min): A0331.D

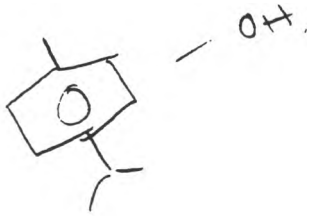
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
115.00	158	139.00	439				
121.95	162	140.15	79				
122.95	497	142.05	45				
123.95	148	146.80	44				
124.95	187	150.20	79				
126.05	122	151.05	299				
132.00	104	152.05	4758				
133.15	74	153.00	659				
135.00	108	153.90	256				
137.00	13288	155.65	56				
138.00	1502	168.05	44				

Scan 601 (14.987 min): A0331.D

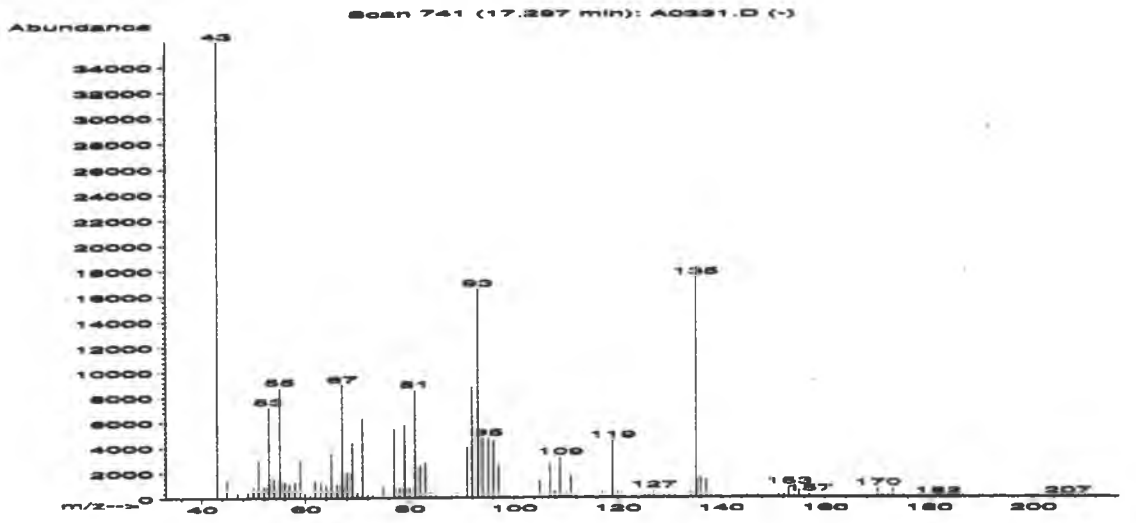
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Pyrazine, 2-methoxy-3-(1-methylethyl)-	152	C8H12N2O	87
2.	Ethanone, 1-(2,4-dihydroxyphenyl)-	152	C8H8O3	80
3.	2-Methyl-1,3-benzoxathiole	152	C8H8OS	72
4.	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	72
5.	Pyrazine, 2-methoxy-3-(1-methylethyl)-	152	C8H12N2O	72
6.	Isodehydroiridodiol	170	C10H18O2	64
7.	2-Methyl-1-(isopropylamino)-1-cyanobuten	152	C9H16N2	64
8.	2-ISOPROPYL-4-METHOXYPYRIMIDINE	152	C8H12N2O	64
9.	1-tert-Butyl-3,4-dimethylpyrazole	152	C9H16N2	64
10.	2,5-DIMETHOXYTOLUENE	152	C9H12O2	59
11.	Ethanone, 1-(2,5-dihydroxyphenyl)-	152	C8H8O3	59
12.	Silane, trimethyl(4-methyl-3-penten-1-yn	152	C9H16Si	53
13.	(E)-4-(2',6',6'-Trimethyl-1',2'-epoxycyc	222	C14H22O2	53
14.	Ethanone, 1-(2,4-dihydroxyphenyl)-	152	C8H8O3	50
15.	1,3-DIAZIN, 6-HYDROXY-2-ISOPROPYL-4-METH	152	C8H12N2O	50
16.	4(1H)-Pyrimidinone, 6-methyl-2-(1-methyl	152	C8H12N2O	50
17.	Thiazolo[5,4-d]pyrimidine	137	C5H3N3S	50
18.	4(1H)-Pyrimidinone, 6-methyl-2-(1-methyl	152	C8H12N2O	50
19.	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	43
20.	2-AMINO-4,5,6,7-D4-BENZIMIDAOLE	133	C7H3D4N3	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	025773-40-4	13395	59	35	1	86	10	54	0	56	9942
2.	*80	000089-84-9	123904	55	39	1	79	15	48	0	49	9882
3.	*72	000000-00-0	13331	51	40	2	83	18	42	0	44	9874
4.	*72	002785-89-9	13455	51	36	2	81	18	42	15	44	9599
5.	*72	025773-40-4	123917	48	61	2	97	16	42	0	44	8819
6.	64	076792-79-5	21459	47	45	1	85	16	37	17	38	9453
7.	*64	066102-53-2	13548	44	66	3	99	20	37	0	40	9351
8.	*64	064958-53-8	13387	23	18	1	88	6	37	3	32	9878
9.	*64	063989-68-4	13551	39	7	0	99	16	37	12	39	8306
10.	*59	024599-58-4	123927	51	39	2	86	21	33	6	40	9655
11.	*59	000490-78-8	13360	47	49	3	66	23	33	9	38	9349
12.	*53	062338-12-9	13564	35	39	1	95	28	28	18	40	9827
13.	53	089128-12-1	44868	43	53	1	99	30	28	0	39	9358
14.	*50	000089-84-9	13359	43	43	1	99	18	25	6	33	9894
15.	*50	000000-00-0	13399	36	49	1	75	18	25	4	34	9891
16.	*50	002814-20-2	123914	36	39	2	80	20	25	1	36	9817
17.	*50	000273-86-9	8217	37	58	3	99	35	25	0	39	9103
18.	*50	002814-20-2	13384	36	49	1	75	18	25	4	34	9891
19.	*43	002785-89-9	123923	49	43	1	59	46	18	0	46	9872
20.	*40	000000-00-0	7100	38	59	3	73	35	16	0	35	9178



Peak 54 Monoterpene (Sulpher containing)



Scan 741 (17.297 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	36023	56.90	1074	68.05	2047	80.00	809
44.95	1420	57.90	1260	69.05	4407	81.00	8561
46.95	406	59.00	3003	70.05	472	82.00	2560
48.95	502	59.90	367	71.05	6324	83.00	2769
49.95	852	60.95	197	72.00	218	84.00	413
50.95	2983	61.90	1419	73.00	249	85.00	352
52.05	962	63.00	1216	74.05	150	88.00	241
52.95	7198	64.00	1036	74.95	845	89.00	412
53.95	1572	65.00	3562	77.05	5449	91.00	4001
55.05	8758	66.10	1119	78.05	838	91.95	8819
56.00	1255	67.10	8997	79.05	5720	93.05	16527

Scan 741 (17.297 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
93.95	4722	109.00	3224	121.00	258	136.10	1663
95.05	4746	110.00	393	123.05	175	137.15	1472
96.05	4545	111.00	1786	125.15	233	138.05	145
97.05	2661	112.00	142	126.00	341	139.00	136
98.00	92	113.00	44	126.95	591	145.00	168
99.00	49	114.00	169	128.90	243	147.05	133
102.05	105	114.95	365	129.90	247	151.05	250
103.05	255	117.05	529	131.00	137	152.05	270
105.00	1350	117.95	261	133.05	25	153.00	846
107.00	2673	119.05	4534	134.10	551	154.05	128
108.00	552	120.05	484	135.15	17456	155.00	567

Scan 741 (17.297 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
157.00	266						
163.15	43						
168.05	86						
170.05	733						
170.95	323						
172.05	183						
173.05	694						
175.05	277						
181.65	34						
206.65	65						

Compounds from Proctor and Gamble A0331.D

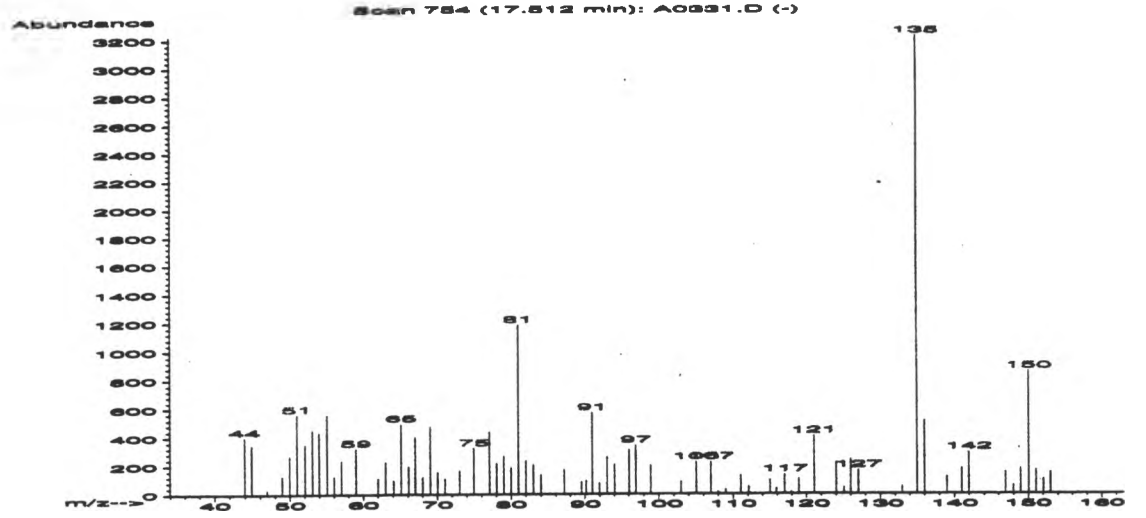
Scan 741 (17.297 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Nerol	154	C10H18O	35
2.	1-P-MENTHEN-8-YL ACETATE	196	C12H20O2	25
3.	CYCLOPENTANE, 1-ACETOXYMETHYL-3-ISOPROPE	196	C12H20O2	25
4.	THUJYL ALCOHOL	154	C10H18O	25
5.	MYRTANYLACETATE	196	C12H20O2	25
6.	Cyclohexanol, 1-methyl-4-(1-methyletheny	154	C10H18O	22
7.	Dihydrocarvyl acetate	196	C12H20O2	17
8.	Linalyl acetate	196	C12H20O2	12
9.	.BETA.-TERPINYL ACETATE	198	C12H22O2	12
10.	trans-Geraniol	154	C10H18O	10
11.	(-)-CURCUPHENOL	218	C15H22O	10
12.	2,3-Hexadiene, 2-methyl-	96	C7H12	10
13.	2-Butenal, 2-ethenyl-	96	C6H8O	9
14.	.beta.-Myrcene	136	C10H16	9
15.	Limonene oxide	152	C10H16O	9
16.	Cyclohexanol, 2-methylene-3-(1-methyleth	196	C12H20O2	9
17.	.beta.-Myrcene	136	C10H16	9
18.	3-Octyne	110	C8H14	9
19.	2,5-OCTADIENE	110	C8H14	9
20.	Cyclohexanamine, N-methyl-	113	C7H15N	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	000106-25-2	124192	47	61	2	66	53	11	0	40	7274
2.	25	000080-26-2	128013	47	66	3	140	53	7	0	35	7302
3.	25	000000-00-0	32953	54	79	2	59	54	7	0	36	6896
4.	25	000513-23-5	124301	47	57	3	86	53	7	0	35	6935
5.	25	000000-00-0	33020	44	67	3	46	54	7	0	35	6940
6.	*22	000138-87-4	124296	34	82	3	53	61	5	0	39	7084
7.	17	020777-49-5	32973	42	76	2	63	53	3	1	29	7167
8.	12	000115-95-7	127992	42	70	2	99	57	2	0	29	7068
9.	12	000000-00-0	33969	44	91	3	51	61	2	0	35	6950
10.	*10	000106-24-1	124201	37	60	2	85	69	1	0	35	6308
11.	10	069301-27-5	42956	57	52	1	35	69	1	3	37	6606
12.	*10	029212-09-7	622	46	25	0	23	78	1	13	40	4028
13.	* 9	020521-42-0	576	33	51	1	31	72	1	0	35	4345
14.	* 9	000123-35-3	8068	44	60	2	112	75	1	0	35	6583
15.	9	001195-92-2	13724	43	50	1	26	73	1	0	37	5794
16.	9	054845-30-6	32974	46	59	1	71	80	1	2	37	6278
17.	* 9	000123-35-3	121970	34	58	3	143	79	1	0	30	6133
18.	9	015232-76-5	2218	49	46	2	36	72	1	0	31	4208
19.	9	000000-00-0	2226	38	60	0	33	75	1	0	33	4046
20.	* 9	000100-60-7	119176	39	54	2	86	78	1	12	37	3753

Peak 55



Scan 754 (17.512 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	401	57.00	233	71.05	110	87.15	173
44.90	345	59.00	322	73.00	166	89.50	88
46.95	30	62.00	112	74.95	326	90.15	96
48.95	128	63.00	226	77.05	442	91.00	573
49.95	266	64.10	98	78.05	218	91.95	77
50.95	562	65.10	495	79.00	270	93.00	262
52.05	349	66.10	196	80.00	188	94.05	208
53.05	452	67.00	403	81.00	1183	96.05	309
53.95	434	68.00	122	82.00	235	96.95	344
55.05	560	69.05	475	83.00	206	98.95	201
56.00	124	70.05	156	84.00	138	102.95	87

Scan 754 (17.512 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.00	225	121.05	410	146.95	153		
107.00	225	124.00	222	148.00	58		
108.00	15	125.05	43	148.95	178		
109.00	30	126.00	242	150.05	859		
111.00	128	127.05	167	151.05	167		
112.10	51	132.95	52	152.05	103		
115.00	98	135.00	3223	153.00	152		
115.90	38	136.00	515				
117.05	138	139.00	122				
117.95	15	140.95	180				
118.95	109	141.95	293				

Compounds from Proctor and Gamble A0331.D

Scan 754 (17.512 min): A0331.D

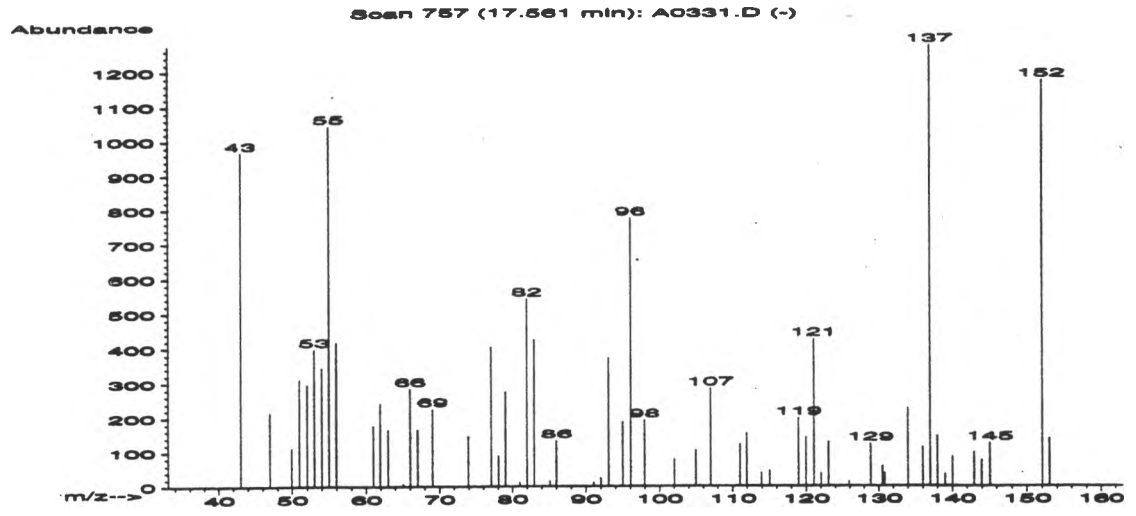
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-ethyl-4,5-dimethyl-	150	C10H14O	62
2.	4-Picolinium, 1-acetamido-, hydroxide, i	150	C8H10N2O	58
3.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	58
4.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	58
5.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	58
6.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	52
7.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	52
8.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	52
9.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	52
10.	Benzene, 1-methoxy-4-(1-methylethyl)-	150	C10H14O	52
11.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	52
12.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	52
13.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	52
14.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	52
15.	1-VINYL-2,6,6-TRIMETHYLCYCLOHEX-1-ENE	150	C11H18	50
16.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	50
17.	Benzothiazole	135	C7H5NS	43
18.	Silane, (chloromethyl)dimethylphenyl-	184	C9H13ClSi	43
19.	1,2-Benzisothiazole	135	C7H5NS	43
20.	2H-1,4-Benzoxazine, 3,4-dihydro-	135	C8H9NO	43

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*62	002219-78-5	12732	70	20	1	76	29	36	14	58	9734
2.	*58	007584-29-4	12544	63	43	3	98	35	32	0	58	9717
3.	*58	000499-75-2	123690	35	60	2	87	29	32	4	43	9772
4.	*58	000499-75-2	123691	54	40	1	76	29	32	0	47	9770
5.	*58	000499-75-2	123692	54	40	1	76	29	32	0	47	9770
6.	*52	000499-75-2	123688	50	53	1	80	33	27	0	46	9749
7.	*52	000089-83-8	12728	45	47	0	67	35	27	0	44	9733
8.	*52	000088-18-6	123670	54	44	1	78	35	27	0	49	9706
9.	*52	000088-18-6	123666	48	52	1	82	35	27	0	46	9724
10.	*52	004132-48-3	12753	52	40	1	86	35	27	0	44	9726
11.	*52	000499-75-2	123687	48	41	1	71	33	27	0	44	9757
12.	*52	000098-54-4	123676	51	45	1	96	35	27	0	44	9721
13.	*52	000499-75-2	123693	63	29	1	72	33	27	28	47	9775
14.	*52	000088-18-6	123665	49	54	2	72	35	27	0	46	9719
15.	*50	005293-90-3	12922	45	59	2	80	32	25	0	40	9777
16.	*50	000088-18-6	12725	35	59	2	71	35	25	0	41	9680
17.	*43	000095-16-9	7530	49	33	0	83	45	18	6	41	9422
18.	43	001833-51-8	27326	58	35	2	99	45	18	0	43	9425
19.	*43	000272-16-2	7531	56	35	2	93	47	18	0	49	9399
20.	*43	005735-53-5	7580	43	57	1	70	48	18	0	44	9441

Compounds from Proctor and Gamble A0331.D

Peak 56



Scan 757 (17.561 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	967	63.00	164	83.00	425	107.00	284
46.95	215	65.05	7	85.10	17	111.00	123
49.95	112	66.00	284	86.00	133	111.95	154
50.95	311	67.00	166	91.05	11	113.90	38
52.00	296	69.05	226	92.00	24	115.00	46
53.00	397	73.95	146	93.05	373	117.05	2
54.00	343	77.05	404	94.95	189	118.95	199
54.95	1044	78.05	89	96.05	774	119.95	144
55.95	415	79.05	275	97.95	193	121.05	426
61.00	177	81.00	11	102.05	79	122.05	38
61.90	242	82.00	542	105.00	105	123.05	129

Scan 757 (17.561 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.95	14	143.95	76				
128.90	124	145.05	126				
130.50	58	152.05	1173				
130.80	37	153.00	139				
134.00	228						
136.00	115						
137.00	1275						
138.00	146						
139.00	35						
140.00	86						
142.95	99						

Compounds from Proctor and Gamble A0331.D

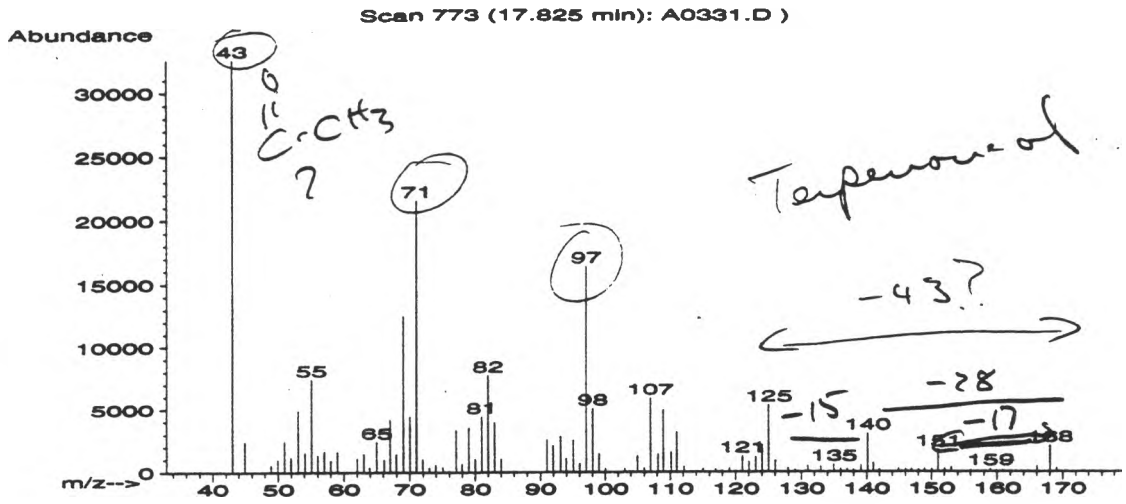
Scan 757 (17.561 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-Fluoro-2,3,5,6-tetramethylbenzene	152	C10H13F	49
2.	2,5-DIMETHOXYTOLUENE	152	C9H12O2	43
3.	.beta.-Cyclocitral	152	C10H16O	38
4.	1H-Inden-1-one, octahydro-7a-methyl-, ci	152	C10H16O	38
5.	2-METHOXY-4,5,6-TRIMETHYLPYRIMIDINE	152	C8H12N2O	30
6.	1,4-Benzenediol, 2,3,5-trimethyl-	152	C9H12O2	27
7.	1,4,5,6-TETRAMETHYL-2-PYRIMIDONE	152	C8H12N2O	27
8.	2,5-DIMETHOXYTOLUENE	152	C9H12O2	25
9.	.beta.-Cyclocitral	152	C10H16O	25
10.	2-OXO-1-METHYL-3-ISOPROPYLPYRAZINE	152	C8H12N2O	25
11.	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	22
12.	Benzenamine, 2-methyl-4-nitro-	152	C7H8N2O2	22
13.	Benzenamine, 2-methyl-5-nitro-	152	C7H8N2O2	22
14.	2(1H)-Naphthalenone, octahydro-, trans-	152	C10H16O	14
15.	Phenol, 5-methoxy-2,3-dimethyl-	152	C9H12O2	14
16.	Benzoic acid, 4-methoxy-	152	C8H8O3	10
17.	Ethanone, 1-(2,4-dihydroxyphenyl)-	152	C8H8O3	10
18.	1-Oxaspiro[2.5]octane, 4,4-dimethyl-8-me	152	C10H16O	10
19.	Benzoic acid, 3-methoxy-	152	C8H8O3	10
20.	8-AZAGUANINE	152	C4H4N6O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	000319-92-6	13573	35	22	0	97	37	23	10	43	8338
2.	*43	024599-58-4	123927	58	44	1	94	47	18	22	49	8330
3.	*38	000432-25-7	123966	60	72	3	85	60	14	0	56	8522
4.	*38	013025-91-7	124002	40	63	0	91	49	14	0	39	7269
5.	*30	065641-61-4	123916	48	74	2	91	57	9	0	46	6673
6.	*27	000700-13-0	13531	50	66	1	90	59	8	1	40	8313
7.	*27	078365-50-1	13402	44	75	1	83	59	8	0	40	8829
8.	*25	024599-58-4	13471	52	61	1	99	62	7	0	46	8368
9.	*25	000432-25-7	13652	58	69	2	111	62	7	0	46	8453
10.	*25	078210-68-1	13403	33	47	0	91	64	7	18	43	8607
11.	*22	002785-89-9	13455	38	55	1	70	64	5	0	39	8334
12.	*22	000099-52-5	13303	47	53	0	65	63	5	5	40	6144
13.	*22	000099-55-8	123857	48	54	0	73	63	5	8	41	6144
14.	*14	016021-08-2	13762	33	102	3	142	66	2	0	39	7318
15.	*14	034883-01-7	13456	36	70	1	91	70	2	0	39	8026
16.	*10	000100-09-4	123886	34	72	1	86	77	1	0	39	5970
17.	*10	000089-84-9	123904	36	59	2	203	80	1	0	39	8020
18.	10	054345-56-1	13767	46	67	1	81	76	1	18	38	7706
19.	*10	000586-38-9	123884	34	68	1	64	78	1	0	39	5906
20.	*10	000134-58-7	13219	37	73	1	91	78	1	13	40	6220

Peak 57



Scan 773 (17.825 min): A0331.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	32560	58.00	891	71.05	21416	82.00	7724
44.95	2396	59.00	1602	71.95	1053	83.00	3954
48.95	535	62.00	1073	72.95	348	84.00	1063
49.95	1002	63.00	1453	73.95	582	91.00	2595
50.95	2488	63.90	378	75.05	410	91.95	2126
51.95	1174	65.00	2432	75.95	111	93.05	2837
53.05	4901	66.15	1003	77.05	3361	93.95	1079
54.05	1550	67.00	4194	77.95	641	95.05	2553
55.05	7421	67.95	1444	79.05	3572	96.05	692
56.00	1340	69.05	12450	80.00	1024	97.05	16301
57.00	1669	70.05	4434	81.00	4453	98.05	5092

Scan 773 (17.825 min): A0331.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.05	1454	115.00	273	127.95	304	141.95	192
100.05	264	116.95	227	129.00	153	144.95	259
103.05	270	117.95	130	131.00	459	146.05	199
105.00	1283	119.05	305	133.00	419	146.95	181
106.00	300	120.05	91	135.00	558	148.05	148
107.00	5898	121.05	1249	136.00	227	148.95	216
108.15	1432	122.05	799	137.00	227	150.05	205
109.00	4965	123.05	1205	138.00	174	151.05	1754
110.15	1584	124.05	2116	139.15	507	152.05	244
111.00	3188	125.05	5349	140.15	3042	153.00	369
112.15	449	126.05	886	141.05	664	156.00	141

Scan 773 (17.825 min): A0331.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
159.00	204						
159.90	100						
160.90	130						
161.90	55						
166.05	426						
168.05	2065						
169.05	296						

Scan 773 (17.825 min): A0331.D

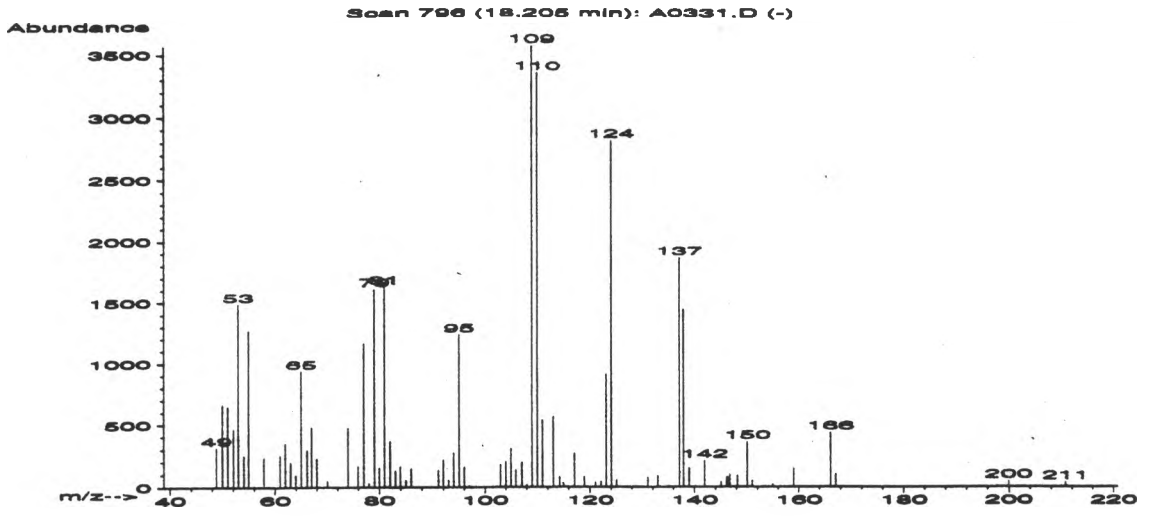
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2,4-Pentanedione, 3-(2-propenyl)-	140	C8H12O2	35
2.	Menthol	156	C10H20O	30
3.	Thiophene, 2-hexyl-	168	C10H16S	25
4.	Thiophene, 2-hexyl-	168	C10H16S	22
5.	Thiophene, 2-hexyl-	168	C10H16S	22
6.	Thiophene, 2-isohexyl-	168	C10H16S	22
7.	CYCLOHEXANE, 2,4-DIISOPROPYL-1,1-DIMETHY	196	C14H28	16
8.	4-ACETONYLCYCLOHEXANONE	154	C9H14O2	14
9.	1,3,4-Trimethyl-1-sila-3-cyclohexene	140	C8H16Si	14
10.	3,3-(D2)MENTH-1-ENE	138	C10H16D2	14
11.	Ethanone, 1-(7-oxabicyclo[4.1.0]hept-1-y	140	C8H12O2	14
12.	Thiophene, 2-methyl-	98	C5H6S	14
13.	2-ACETYL-1,4,5,6-TETRAHYDROPYRIDINE	125	C7H11NO	11
14.	Bicyclo[2.2.1]heptan-2-ol, 3,3-dimethyl-	140	C9H16O	11
15.	1,3-Propanediol, 2-(bromomethyl)-2-(hydr	198	C5H11BrO3	10
16.	2-(2-Oxopropyl)-1-cyclopentanone	140	C8H12O2	10
17.	3-t-Butyl-2-(5H)-furanone	140	C8H12O2	10
18.	2,5-DIMETHYLCYCLOHEXANOL	128	C8H16O	10
19.	1-ACETYL-2(2-PROPANONE)-CYCLOPENTANE	168	C10H16O2	10
20.	7-Oxabicyclo[4.1.0]heptane, 3-methyl-	112	C7H12O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	003508-78-9	122443	35	49	3	186	51	11	0	39	6373
2.	*30	000089-78-1	15580	53	56	2	63	56	9	0	49	7849
3.	*25	018794-77-9	125767	35	36	0	36	65	7	22	43	5677
4.	*22	018794-77-9	125765	34	36	0	35	65	5	0	39	5693
5.	*22	018794-77-9	125766	34	36	0	35	65	5	0	39	5694
6.	*22	004861-59-0	20531	43	30	0	47	65	5	11	39	5713
7.	16	000000-00-0	33195	46	55	1	42	56	3	3	37	7798
8.	14	086428-59-3	14506	45	52	1	91	69	2	0	39	5562
9.	*14	078698-05-2	9315	35	21	0	21	69	2	0	41	5579
10.	*14	005206-77-9	8793	45	44	0	29	69	2	16	40	6257
11.	*14	015121-01-4	9259	46	46	3	124	68	2	0	40	6012
12.	*14	000554-14-3	117690	33	55	0	50	69	2	0	41	5689
13.	*11	000000-00-0	5002	43	44	0	34	80	2	0	44	3683
14.	*11	005957-68-6	9413	44	46	0	19	78	2	0	44	5180
15.	10	019184-65-7	33456	44	77	1	60	75	1	0	39	7054
16.	*10	060415-94-3	9207	35	57	2	98	74	1	0	39	5649
17.	*10	063711-18-2	9195	33	37	0	18	78	1	0	41	5418
18.	*10	000000-00-0	6019	33	37	0	39	74	1	0	41	7261
19.	10	000000-00-0	20372	47	36	1	81	77	1	1	38	2943
20.	*10	036099-51-1	2628	37	61	0	34	74	1	0	41	5471

No m/e 170 coeluting with peak. Sulpher unlikely.

Peak 58



Scan 796 (18.205 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.80	312	62.00	350	78.00	27	93.00	53
49.95	662	63.00	192	79.05	1607	94.00	276
50.95	646	63.95	95	80.00	149	95.05	1237
52.05	463	65.00	936	81.00	1626	96.00	155
53.00	1486	66.10	296	82.00	361	97.00	10
54.05	250	67.00	478	83.00	129	102.95	176
55.00	1268	67.95	225	83.95	157	104.00	202
56.00	10	70.00	46	85.00	51	105.00	308
56.95	5	73.95	474	85.95	144	105.95	134
57.85	234	75.95	164	91.10	134	107.10	195
61.00	249	77.00	1162	92.00	216	108.00	16

Scan 796 (18.205 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.00	3568	124.05	2804	146.30	79		
110.00	3347	125.05	55	146.70	98		
111.00	538	131.00	78	148.20	91		
113.00	565	133.00	88	150.05	359		
114.25	82	135.05	6	151.05	48		
115.00	24	137.15	1864	155.00	19		
117.00	269	138.00	1443	159.00	144		
118.95	80	139.00	148	166.05	435		
121.00	33	141.95	208	167.05	97		
122.05	43	145.05	40	199.95	45		
123.05	910	146.05	78	210.75	34		

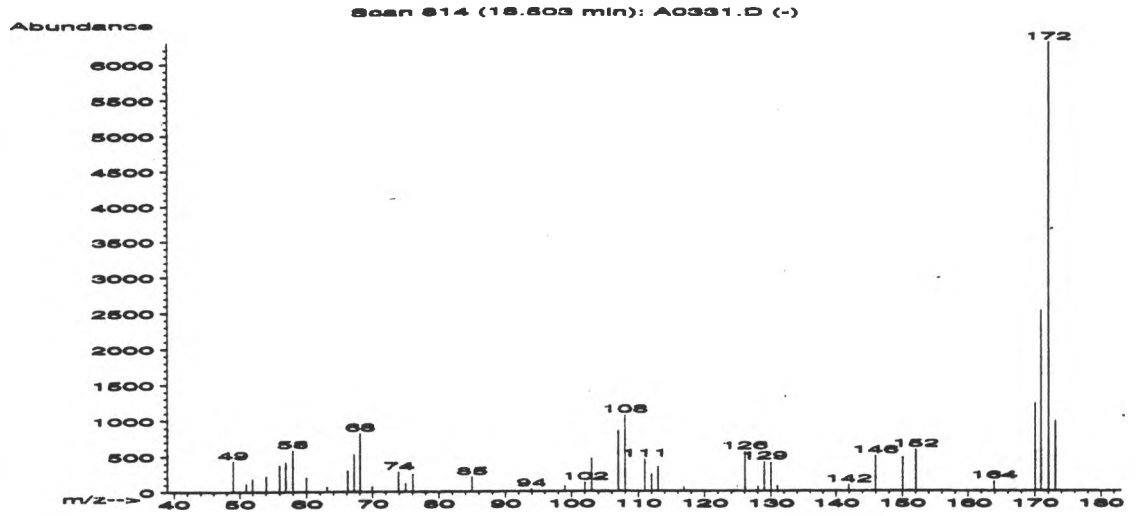
Scan 796 (18.205 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-Cyclopenten-1-one, 3,4,5-trimethyl-	124	C8H12O	43
2.	2-(2-Hydroxypropyl)-3-furancarbaldehyde	154	C8H10O3	38
3.	Phenol, 4-ethoxy-	138	C8H10O2	35
4.	1,4-Benzenediol	110	C6H6O2	35
5.	1-METHYL-2-PYRROLECARBOXALDEHYDE	109	C6H7NO	22
6.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	20
7.	2-Furancarboxaldehyde, 5-methyl-	110	C6H6O2	15
8.	Benzene, 1-fluoro-2-methyl-	110	C7H7F	14
9.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	14
10.	Phenol, 4-methoxy-	124	C7H8O2	14
11.	Phenol, 4-methoxy-	124	C7H8O2	14
12.	1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	14
13.	Phenol, 2-methoxy-	124	C7H8O2	14
14.	Phenol, 2-methoxy-	124	C7H8O2	14
15.	2-Furancarboxaldehyde, 5-methyl-	110	C6H6O2	11
16.	2-(2',2',2'-D3-ETHYL)PYRIDINE	107	C7H6D3N	11
17.	1,3-Hexadiene, 3-ethyl-2,5-dimethyl-	138	C10H18	10
18.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	10
19.	Pyridine, 4-methoxy-	109	C6H7NO	10
20.	Phenol, 2-methoxy-	124	C7H8O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	055683-21-1	4786	54	46	1	80	42	18	13	40	7409
2.	38	087773-71-5	14309	44	39	0	82	46	14	2	41	8104
3.	*35	000622-62-8	122228	43	59	3	93	51	11	1	40	6202
4.	*35	000123-31-9	118840	49	52	2	93	52	11	12	39	5713
5.	22	001192-58-1	2034	47	53	0	62	65	5	12	41	6225
6.	*20	001072-91-9	118843	62	36	2	93	70	4	0	56	7459
7.	*15	000620-02-0	118825	67	41	1	70	72	2	15	50	7509
8.	*14	000095-52-3	118845	36	45	2	99	66	2	1	40	7234
9.	*14	001072-91-9	118842	38	46	1	95	70	2	11	40	7530
10.	*14	000150-76-5	120386	36	56	1	86	67	2	0	39	7392
11.	*14	000150-76-5	120385	36	57	1	86	68	2	1	40	7341
12.	*14	000931-36-2	2142	43	37	2	99	70	2	13	40	6877
13.	*14	000090-05-1	120383	43	53	1	68	68	2	0	39	7345
14.	*14	000090-05-1	120379	41	51	2	95	70	2	0	39	7299
15.	*11	000620-02-0	2126	49	65	2	81	73	2	0	44	7430
16.	*11	000000-00-0	1816	44	65	0	86	71	2	0	44	7531
17.	*10	062338-07-2	8753	50	58	2	96	72	1	18	39	6197
18.	*10	001072-91-9	2139	46	53	2	88	80	1	0	40	6482
19.	*10	000620-08-6	2056	34	61	3	92	78	1	0	39	6287
20.	*10	000090-05-1	4705	33	61	1	86	71	1	1	40	7196

Peak 59a



Scan 814 (18.503 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
48.95	435	68.05	823	108.00	1068	145.95	493
50.95	114	69.95	68	111.00	449	150.05	477
51.95	182	73.95	284	112.00	240	151.00	15
54.05	221	75.00	121	113.00	344	152.05	587
56.00	377	76.05	249	116.95	56	163.90	141
56.90	419	85.00	204	126.05	552	170.05	1233
57.95	587	93.95	39	128.05	67	170.95	2517
59.95	199	99.05	76	129.00	414	172.05	6297
63.00	70	102.05	129	130.00	406	173.05	980
66.10	299	103.05	468	131.00	76		
67.10	528	107.00	854	141.95	86		

Compounds from Proctor and Gamble A0331.D

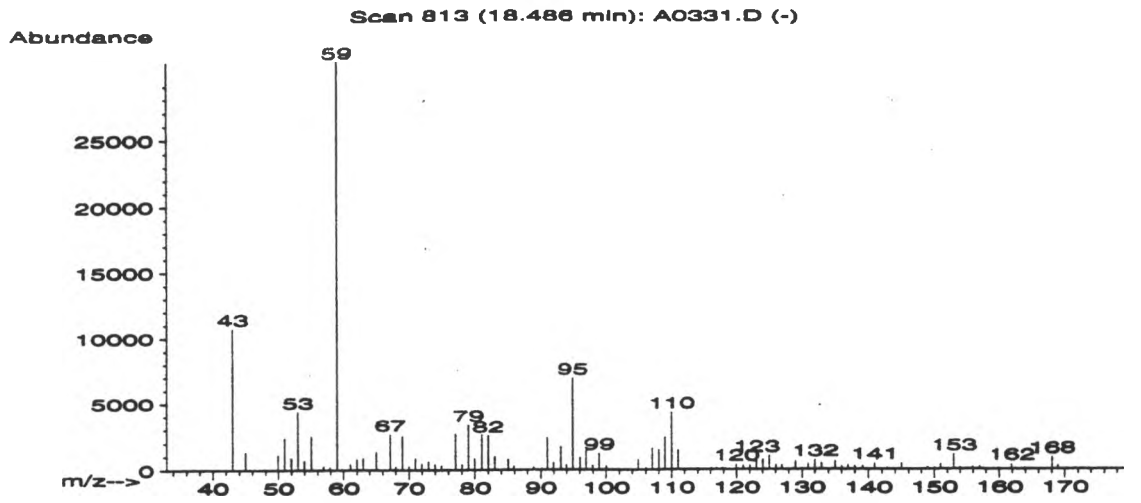
Scan 814 (18.503 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	59
2.	2,2'-OXYDIPYRIDINE	172	C10H8N2O	40
3.	1-METHYL-4-METHOXYNAPHTHALENE	172	C12H12O	38
4.	1-METHOXY-8-METHYLNAPHTHALENE	172	C12H12O	35
5.	1-METHYL-2-METHOXYNAPHTHALENE	172	C12H12O	23
6.	1H-Pyrazole, 3,5-dimethyl-1-phenyl-	172	C11H12N2	17
7.	2-Naphthalenecarboxylic acid	172	C11H8O2	17
8.	2-Naphthalenecarboxylic acid	172	C11H8O2	17
9.	2-Naphthalenecarboxylic acid	172	C11H8O2	17
10.	1-Naphthalenecarboxylic acid	172	C11H8O2	17
11.	1-METHOXY-2-METHYLNAPHTHALENE	172	C12H12O	17

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	000321-60-8	22421	44	56	1	99	24	33	0	40	9613
2.	*40	053258-94-9	22256	30	46	1	71	31	16	8	35	9458
3.	*38	000000-00-0	22446	35	81	2	92	50	14	0	39	9137
4.	*35	000000-00-0	22443	35	84	2	99	52	11	0	39	8891
5.	*23	000000-00-0	22444	29	87	2	99	50	6	0	27	9096
6.	*17	001131-16-4	22397	29	92	3	99	53	3	0	27	9235
7.	*17	000093-09-4	126216	29	77	1	87	52	3	0	29	8957
8.	*17	000093-09-4	126215	30	79	1	81	53	3	0	27	8890
9.	*17	000093-09-4	126214	29	79	2	99	52	3	0	29	8930
10.	*17	000086-55-5	22387	29	83	1	70	52	3	0	29	9024
11.	*17	000000-00-0	22442	29	91	2	82	52	3	0	29	8891

Peak 59b



Scan 813 (18.486 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	10737	61.00	420	73.95	396	85.90	268
44.95	1312	62.00	782	74.95	328	88.90	195
49.95	1098	63.00	851	76.00	56	90.15	110
50.95	2374	65.00	1317	77.05	2681	91.00	2393
51.95	892	67.15	2661	78.05	407	91.95	521
52.95	4384	68.00	258	79.05	3379	93.05	1745
53.95	722	68.95	2522	80.00	826	93.95	365
55.05	2529	69.95	248	81.00	2642	94.95	6938
56.90	260	70.95	851	82.00	2556	96.05	898
57.90	198	71.95	442	83.00	982	96.95	1491
59.00	30792	72.95	614	85.00	770	97.95	329

Scan 813 (18.486 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.95	1233	116.95	113	129.95	80	144.95	428
100.05	284	117.80	97	130.90	395	148.95	176
104.90	731	119.95	351	132.00	685	150.05	138
106.00	132	121.05	264	133.00	478	150.95	363
107.00	1584	122.05	269	135.00	620	153.00	1085
108.00	1478	123.05	1003	136.00	194	154.00	133
109.00	2432	124.05	716	137.00	321	155.90	181
110.00	4310	125.05	1002	138.00	236	157.00	170
111.00	1426	126.05	313	139.15	253	159.00	36
114.00	77	126.95	327	140.95	441	161.90	381
116.15	94	129.00	557	142.80	130	163.90	112

Scan 813 (18.486 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
168.05	883						
168.95	276						

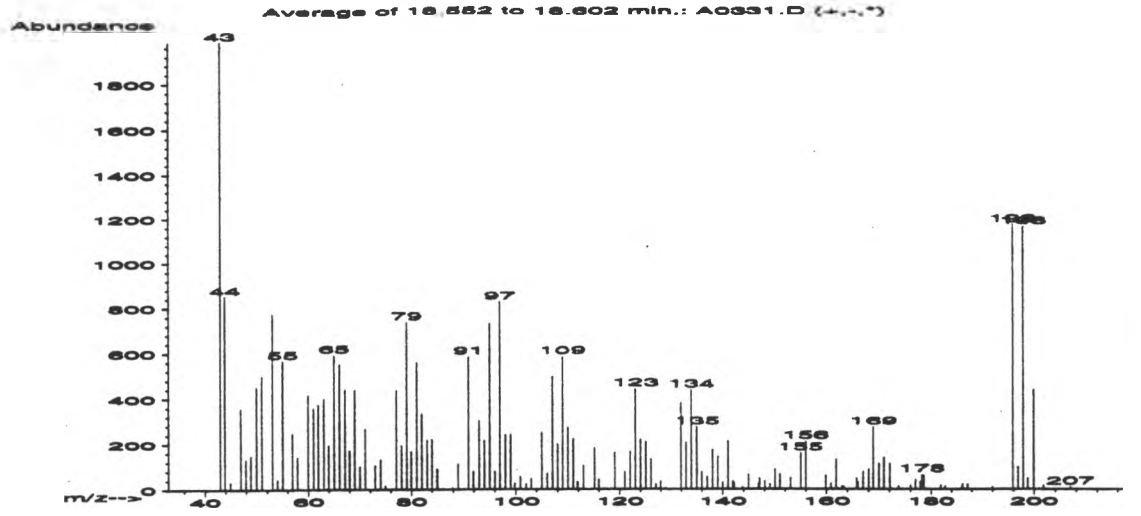
Scan 813 (18.486 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	8-HYDROXYCARVOTANACETONE	168	C10H16O2	56
2.	Cyclooctanemethanol, .alpha.,.alpha.-dim	170	C11H22O	40
3.	5-HYDROXY-4-HYDROXYMETHYL-1-(1-HYDROXY-1	186	C10H18O3	33
4.	1,2,4-Thiadiazole, 5-chloro-	120	C2HClN2S	33
5.	DIHYDRO-TERPINEOL	156	C10H20O	25
6.	3-Octyne	110	C8H14	10
7.	6-Octenoic acid, 3,7-dimethyl-, methyl e	184	C11H20O2	8
8.	8-Heptadecyne, 1-bromo-	314	C17H31Br	7
9.	2-Cyclohexen-1-one, 3-(hydroxymethyl)-6-	168	C10H16O2	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	56	007712-46-1	20525	41	39	0	80	15	30	10	37	9650
2.	40	016624-06-9	21624	48	35	1	69	32	16	8	33	9649
3.	33	087096-72-8	28414	33	90	3	81	31	10	0	20	9690
4.	33	038362-15-1	3994	33	78	3	87	31	10	0	22	9822
5.	25	000000-00-0	15606	33	44	0	89	41	7	0	25	9622
6.	*10	015232-76-5	2218	33	33	0	24	79	1	16	39	2490
7.	8	002270-60-2	27517	42	56	1	39	67	1	0	29	6050
8.	7	056599-94-1	78249	40	97	1	28	77	1	0	24	2445
9.	6	055955-54-9	20397	37	68	1	36	79	1	0	18	1881

Peak 59c Trichlorophenol (not clean)



Average of 18.552 to 18.602 min.: A0331.D
Converted from RTE data file: >A0331:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1985	56.90	247	68.95	438	82.00	335
43.90	853	57.90	142	69.95	100	83.05	217
44.95	31	59.95	416	71.00	266	83.95	222
46.95	357	61.00	357	72.95	105	84.95	90
47.95	132	61.95	373	74.00	132	85.95	2
48.85	147	63.00	399	74.95	17	87.90	9
49.95	450	63.90	195	77.05	436	88.95	111
50.95	498	65.00	591	78.05	194	90.10	3
53.00	774	66.05	550	79.05	737	91.00	583
54.00	43	67.10	439	79.95	168	91.95	79
55.00	566	68.00	170	81.00	558	93.00	304

Average of 18.552 to 18.602 min.: A0331.D
Converted from RTE data file: >A0331:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
94.00	214	106.05	70	119.05	162	132.95	206
95.00	730	107.00	496	121.00	78	133.95	438
96.00	79	108.00	200	122.00	166	135.00	275
96.95	826	109.00	585	123.05	442	136.00	76
98.00	242	110.05	274	124.05	220	137.05	56
99.00	244	111.05	223	125.05	209	138.10	174
99.80	28	111.90	33	126.05	132	139.10	145
100.85	56	113.00	104	127.00	23	140.00	31
101.95	24	115.10	183	127.95	36	141.00	213
102.95	46	116.00	43	128.95	5	141.95	36
104.95	250	116.95	2	131.95	380	142.20	29

Average of 18.552 to 18.602 min.: A0331.D
Converted from RTE data file: >A0331:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.80	10	159.90	61	170.95	141	186.15	24
144.95	65	160.90	26	172.05	113	187.15	23
146.80	25	161.90	131	173.70	16	191.95	12
147.05	49	163.00	13	176.05	19	195.95	1172
148.05	38	163.40	10	176.95	43	196.95	99
149.05	23	165.80	49	177.90	35	197.95	1163
150.05	87	166.05	33	178.20	64	198.80	49
151.00	66	167.00	78	178.60	59	199.95	439
153.05	50	168.05	89	181.90	19	201.75	17
154.95	161	168.95	275	182.75	14	206.90	11
155.95	212	170.00	113	185.90	12		

Compounds from Proctor and Gamble A0331.D

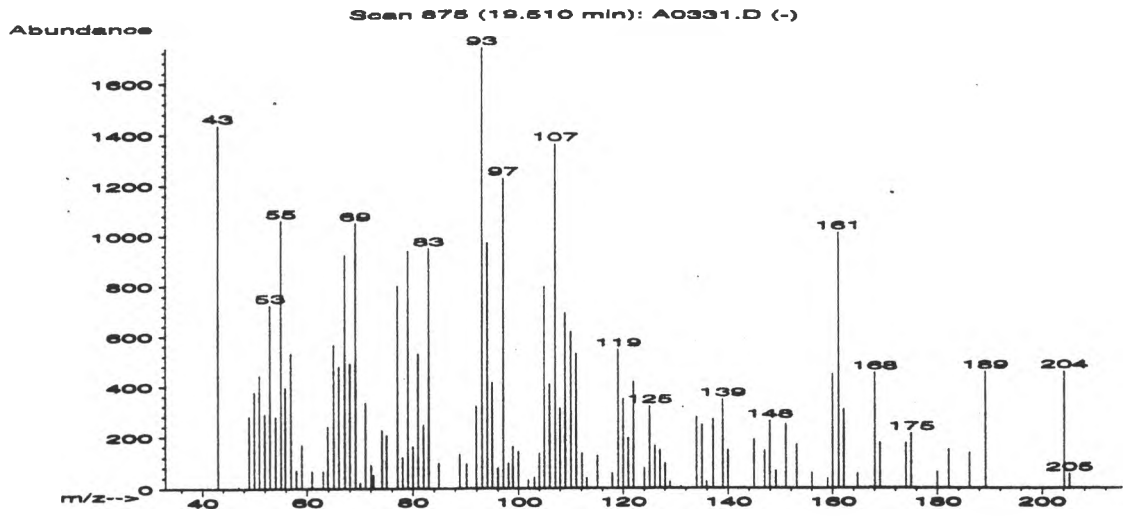
Average of 18.552 to 18.602 min.: A0331.D
Converted from RTE data file: >A0331:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2,4,5-trichloro-	196	C6H3Cl3O	55
2.	2,3,5-Trichlorophenol	196	C6H3Cl3O	53
3.	Phenol, 2,3,4-trichloro-	196	C6H3Cl3O	42
4.	Phenol, 2,4,5-trichloro-	196	C6H3Cl3O	42
5.	Phenol, 2,4,5-trichloro-	196	C6H3Cl3O	38
6.	Propanedinitrile, dimethyl-	94	C5H6N2	38
7.	Phenol, 2,4,5-trichloro-	196	C6H3Cl3O	38
8.	Phenol, 2,3,6-trichloro-	196	C6H3Cl3O	38
9.	3-AMINO-2,4,6-TRICHLOROPYRIDINE	196	C5H3Cl3N2	35
10.	Phenol, 2,4,6-trichloro-	196	C6H3Cl3O	35
11.	Phenol, 2,4,6-trichloro-	196	C6H3Cl3O	30
12.	5-Hexen-3-yn-2-ol, 2-methyl-	110	C7H10O	27
13.	Phenol, 2,3,4-trichloro-	196	C6H3Cl3O	27
14.	Phenol, 2,4,6-trichloro-	196	C6H3Cl3O	25
15.	2,3,5-Trichlorophenol	196	C6H3Cl3O	22
16.	4-Cyclopentene-1,3-diol, trans-	100	C5H8O2	22
17.	3,4,5-Trichlorophenol	196	C6H3Cl3O	20
18.	Phenol, 2,4,6-trichloro-	196	C6H3Cl3O	16
19.	Phenol, 2,3,6-trichloro-	196	C6H3Cl3O	16
20.	Phenol, 2,4,5-trichloro-	196	C6H3Cl3O	15

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*55	000095-95-4	127932	90	60	2	52	62	29	0	92	8651
2.	*53	000933-78-8	127925	93	65	1	54	58	28	0	90	8868
3.	*42	015950-66-0	32529	83	76	2	59	57	17	0	80	8781
4.	*42	000095-95-4	127930	84	60	1	57	59	17	0	80	8805
5.	*38	000095-95-4	127931	83	78	1	54	59	14	0	62	8916
6.	*38	007321-55-3	464	34	78	2	114	48	14	0	39	4236
7.	*38	000095-95-4	127929	90	68	1	59	59	14	0	56	8952
8.	*38	000933-75-5	127928	81	78	2	50	58	14	0	53	9114
9.	*35	000000-00-0	32520	82	64	2	59	70	11	37	64	7786
10.	*35	000088-06-2	32534	67	67	2	59	69	11	0	64	8604
11.	*30	000088-06-2	127934	82	74	2	56	57	9	0	49	8930
12.	27	000690-94-8	2158	45	56	1	99	57	8	16	38	3801
13.	*27	015950-66-0	127924	60	89	2	41	57	8	0	41	8969
14.	*25	000088-06-2	127935	79	89	2	50	65	7	0	49	8896
15.	*22	000933-78-8	32530	46	89	1	40	65	5	0	40	8856
16.	*22	000694-47-3	1096	34	78	2	76	64	5	0	39	3803
17.	*20	000609-19-8	127926	64	74	1	57	66	4	0	58	8422
18.	*16	000088-06-2	127933	74	86	2	51	56	3	6	37	9074
19.	*16	000933-75-5	32532	57	83	2	45	56	3	0	35	9124
20.	*15	000095-95-4	32533	58	68	1	59	74	2	0	56	8242

Peak 60a



Scan 875 (19.510 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1436	57.95	70	71.00	336	83.00	948
46.95	9	59.00	168	72.05	90	84.00	2
48.95	282	60.95	66	72.45	51	84.95	98
49.95	379	63.00	66	74.05	226	88.90	132
50.95	443	63.90	241	74.95	206	90.15	95
52.00	291	65.00	566	77.05	800	91.95	320
53.00	723	66.00	480	78.00	121	93.05	1736
54.10	279	67.10	922	79.05	938	94.05	969
55.05	1061	68.05	490	80.00	162	95.00	415
55.90	395	69.05	1051	81.00	529	96.05	79
56.95	531	69.95	21	82.00	247	97.05	1223

Scan 875 (19.510 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.05	98	110.00	619	125.05	321	140.00	145
98.95	162	111.00	531	126.05	165	142.95	2
99.95	143	112.10	136	127.05	147	144.95	189
101.90	31	113.05	39	128.05	96	147.00	145
103.05	42	115.10	127	128.95	25	147.95	264
104.00	136	117.95	57	131.00	7	149.05	67
105.00	798	119.05	548	134.00	278	151.00	250
106.00	411	120.05	350	135.10	246	153.00	170
107.05	1359	121.00	195	135.95	25	155.95	60
108.00	314	122.00	419	137.15	271	159.00	38
109.00	694	124.05	78	139.00	348	160.00	449

Scan 875 (19.510 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
161.15	1013	204.15	460				
162.15	309	205.15	54				
164.75	56						
168.05	455						
169.05	176						
174.05	176						
175.05	214						
180.00	63						
182.15	149						
186.15	137						
189.15	459						

Compounds from Proctor and Gamble A0331.D

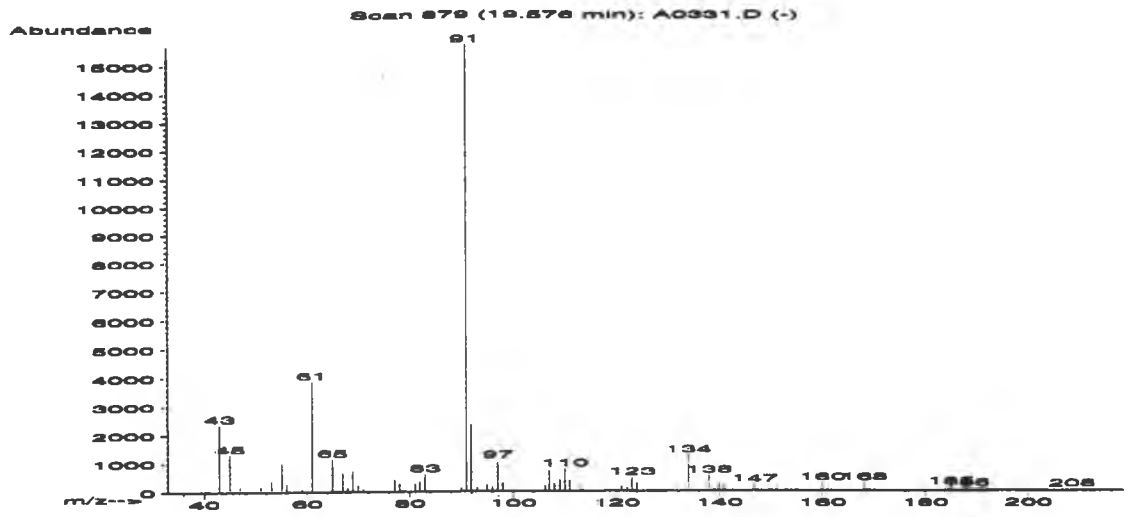
Scan 875 (19.510 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	.beta.-Bisabolene	204	C15H24	49
2.	Bicyclo[6.1.0]non-1-ene	122	C9H14	43
3.	(+)-Aromadendrene	204	C15H24	38
4.	3,5-Hexadien-2-ol, 2-methyl-	112	C7H12O	38
5.	Junipene	204	C15H24	38
6.	Junipene	204	C15H24	38
7.	.beta.-Bisabolene	204	C15H24	25
8.	1,2-Cyclononadiene	122	C9H14	25
9.	2-Phenylethyl-1,1,2,2-d4-amine	121	C8H7D4N	25
10.	Junipene	204	C15H24	22
11.	Patchoulene	204	C15H24	18
12.	1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-	204	C15H24	15
13.	Junipene	204	C15H24	14
14.	.gamma.-Gurjunene	204	C15H24	11
15.	4-BORAPERHYDROINDANE	122	C8H15B	11
16.	3-METHYL-1-PHENYLTRIAZENE	135	C7H9N3	11
17.	Isolongifolene	204	C15H24	11
18.	Ethanone, 1-(1H-pyrrol-2-yl)-	109	C6H7NO	11
19.	Ethanone, 1-(1H-pyrrol-2-yl)-	109	C6H7NO	11
20.	(+)-Aromadendrene	204	C15H24	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	000495-61-4	128663	86	52	1	146	62	23	0	87	8037
2.	*43	002570-06-1	4491	64	64	2	91	50	18	0	44	8046
3.	*38	000489-39-4	128755	67	84	3	126	63	14	0	64	8369
4.	*38	000926-38-5	2590	74	46	1	62	64	14	37	66	4982
5.	*38	000475-20-7	128707	95	78	1	50	63	14	0	66	8290
6.	*38	000475-20-7	128709	59	92	2	125	60	14	0	56	8535
7.	*25	000495-61-4	128662	68	65	3	201	78	7	0	76	7720
8.	*25	001123-11-1	4473	52	84	2	53	61	7	25	45	4506
9.	*25	000000-00-0	4245	62	44	0	95	65	7	18	47	6770
10.	*22	000475-20-7	128708	67	103	2	61	63	5	0	41	8320
11.	*18	001405-16-9	36716	69	87	2	47	68	3	29	47	7435
12.	*15	003853-83-6	128745	61	82	0	44	78	2	0	56	8257
13.	*14	000475-20-7	128710	77	90	1	59	66	2	0	42	8107
14.	*11	022567-17-5	36700	74	95	2	56	75	2	25	45	7508
15.	*11	000000-00-0	4452	48	65	0	45	76	2	0	46	5249
16.	*11	000000-00-0	7536	50	58	2	85	71	2	0	46	6261
17.	*11	001135-66-6	128736	58	94	1	41	76	2	0	46	6437
18.	*11	001072-83-9	118780	35	55	0	50	72	2	2	43	4186
19.	*11	001072-83-9	2036	35	54	0	51	72	2	14	43	4183
20.	*11	000489-39-4	128754	64	103	1	52	75	2	12	47	7806

Peak 60b



Scan 879 (19.576 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2355	63.00	86	82.00	334	106.15	178
44.95	1289	65.00	1131	83.00	604	107.00	708
46.95	166	67.00	635	90.00	128	108.00	255
50.00	45	68.00	127	91.00	15677	109.00	386
50.95	169	68.95	714	91.95	2354	110.00	765
51.95	38	69.95	212	93.05	119	111.00	354
53.00	355	71.00	89	94.95	218	113.00	168
55.05	988	74.95	44	96.00	132	115.05	19
56.00	255	77.05	400	97.00	1074	121.00	177
59.00	93	78.05	265	98.05	281	122.10	109
61.00	3844	81.00	245	105.00	70	123.05	468

Scan 879 (19.576 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.00	267	151.05	170	208.40	38		
133.00	44	153.00	114				
134.00	1249	155.00	99				
136.00	20	160.00	258				
137.10	117	161.00	135				
138.00	519	168.00	254				
139.05	59	168.95	127				
140.00	226	169.95	23				
140.95	202	181.15	94				
146.80	191	185.00	117				
150.05	123	188.00	54				

Compounds from Proctor and Gamble A0331.D

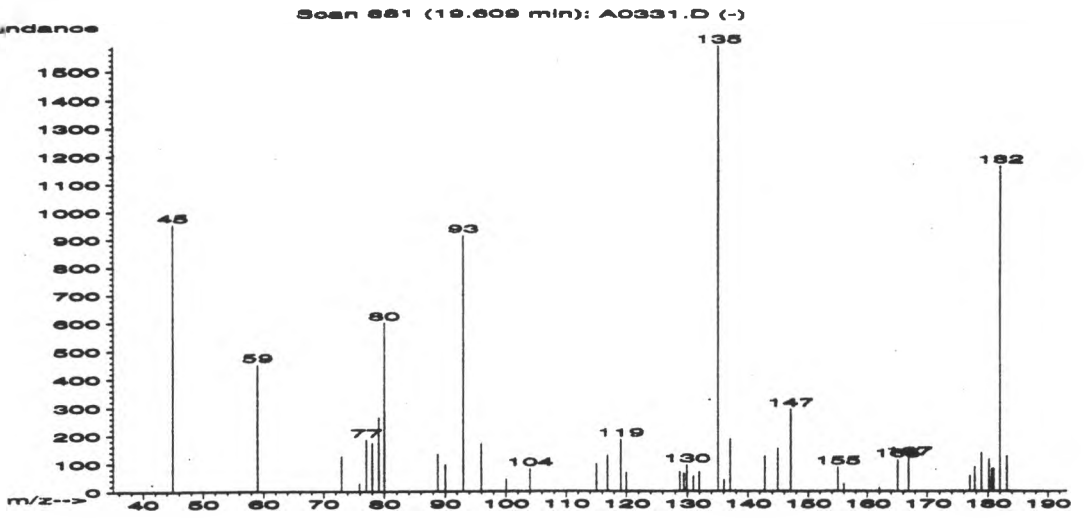
Scan 879 (19.576 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzene, butyl-	134	C10H14	9
2.	Benzene, butyl-	134	C10H14	7
3.	Benzene, 1,1'-[1,4-butanediylbis(oxymeth	270	C18H22O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.*	9	000104-51-8	121602	32	37	0	25	74	1	0	33	9272
2.*	7	000104-51-8	121599	30	40	1	27	74	1	0	29	9055
3.	7	006282-65-1	132209	36	61	2	52	74	1	0	25	9258

Peak 60c



Scan 881 (19.609 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.95	955	95.95	170	131.90	70	165.05	112
59.00	451	100.05	43	135.10	1587	166.95	119
72.95	126	104.00	81	136.05	39	176.95	54
75.90	28	115.05	98	137.05	188	177.75	87
77.05	185	116.95	128	137.95	3	178.90	137
78.00	174	119.05	186	142.80	125	180.15	114
79.05	265	120.00	66	144.95	152	180.65	80
80.00	599	128.75	70	147.05	293	180.90	81
88.75	133	129.40	63	155.00	86	182.00	1160
90.00	96	129.90	94	156.00	25	183.15	125
93.00	912	130.95	53	162.00	14		

Compounds from Proctor and Gamble A0331.D

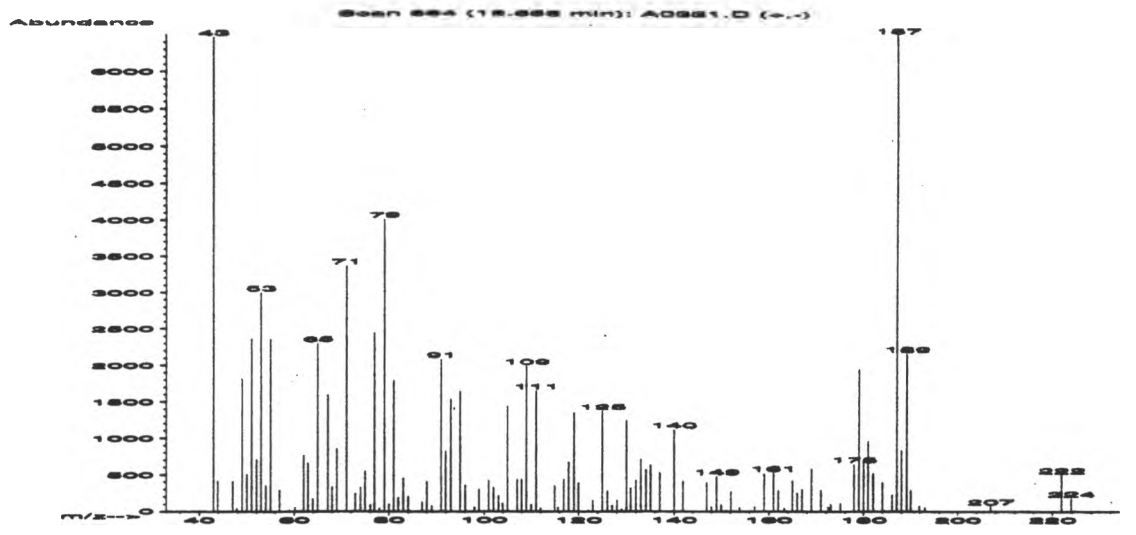
Scan 881 (19.609 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzoic acid, 2,4-dimethoxy-	182	C9H10O4	25
2.	Benzenamine, 2-methoxy-5-methyl-4-nitro-	182	C8H10N2O3	14
3.	1,2-Butanediol, 2-phenyl-, 1-carbamate	209	C11H15NO3	10
4.	1,1'-Biphenyl, 3,3'-dimethyl-	182	C14H14	9
5.	2-Aziridinone, 1-(1-adamantyl)-3-(1-meth	273	C18H27NO	8
6.	3,4-DIETHYLPHENOL	150	C10H14O	8
7.	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	182	C9H10O4	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*25	000091-52-1	26388	47	87	1	88	53	7	2	37	7831
2.	*14	000134-19-0	26332	34	113	0	59	67	2	0	41	5904
3.	10	000050-19-1	38948	36	91	2	74	64	1	0	22	6971
4.	* 9	000612-75-9	127055	35	68	1	67	77	1	0	30	4650
5.	8	026905-18-0	64696	34	99	1	77	69	1	0	21	6660
6.	8	000875-85-4	12892	33	65	1	77	69	1	0	22	6472
7.	* 7	000134-96-3	26404	28	93	2	68	80	1	0	29	5169

Peak 61



Scan 884 (19.659 min): A0331.D

Modified:added subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	6457	56.90	285	72.90	244	84.00	197
43.90	416	59.00	17	74.00	330	86.95	130
46.95	409	60.15	56	75.00	548	88.00	412
47.80	39	61.95	763	76.05	94	89.00	77
48.95	1809	62.95	655	76.95	2431	91.00	2074
49.95	507	63.95	171	78.00	44	91.95	824
50.95	2362	65.00	2288	79.05	3990	93.00	1532
51.95	707	67.10	1586	80.00	99	95.00	1638
52.95	2994	68.00	330	81.00	1783	96.05	358
53.95	353	69.00	853	82.00	184	97.95	62
55.00	2356	71.00	3352	83.00	451	98.95	299

Scan 884 (19.659 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
100.95	416	115.00	347	128.05	154	146.95	388
102.00	323	115.75	59	129.00	28	148.00	59
103.05	213	116.95	436	130.00	1235	149.05	471
103.95	108	118.00	667	130.90	320	150.00	93
105.00	1439	119.05	1339	132.00	423	151.10	13
107.00	439	120.00	389	133.00	706	152.05	267
108.00	442	122.05	18	134.10	565	153.90	46
109.00	1981	123.00	154	135.05	627	157.05	67
110.00	98	125.00	1363	137.00	525	159.00	508
111.05	1643	126.05	272	140.00	1112	161.00	518
112.00	49	127.05	86	141.95	409	162.00	280

Scan 884 (19.659 min): A0331.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.25	42	179.95	691	207.00	68		
164.95	414	180.95	953	221.95	495		
165.95	248	182.00	515	223.95	175		
167.00	294	184.00	390				
169.00	576	186.00	223				
171.00	286	187.00	6497				
172.45	56	188.00	832				
173.00	100	189.10	2137				
175.10	113	190.00	281				
177.95	635	191.80	78				
178.95	1928	192.95	54				

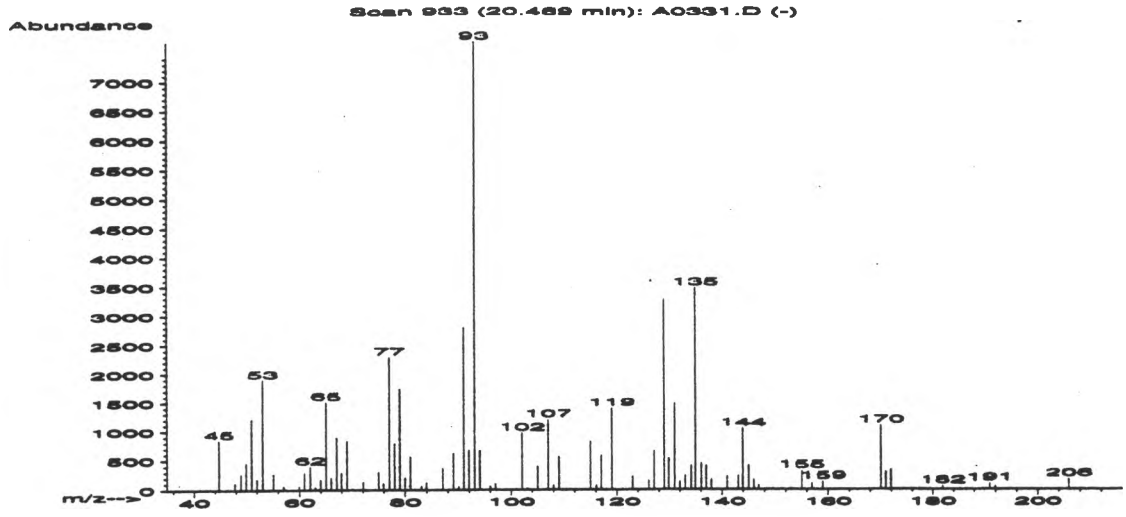
Scan 885 (19.676 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3-Quinolinecarboxylic acid, 1,2-dihydro-	205	C10H7NO4	23
2.	5-Hexen-3-yn-2-ol, 2-methyl-	110	C7H10O	12
3.	2-DEUTEROXYDIPHENYL ETHER	186	C12H9DO2	10
4.	2(1H)-Quinolinone, 4-acetyl-	187	C11H9NO2	10
5.	A,A,A-TRIFLUORO-O-TOLYL ISOCYANATE	187	C8H4F3NO	10
6.	2-Propenoic acid, 3-(1H-indol-3-yl)-	187	C11H9NO2	10
7.	2,6-DICHLOROPHENYL ISOCYANATE	187	C7H3Cl2NO	10
8.	Benzene, 1,2-dichloro-3-isocyanato-	187	C7H3Cl2NO	10
9.	Methyl 2-carboxyridine-3-carboxylate	187	C8H13NO4	10
10.	Benzene, 1,4-dichloro-2-isocyanato-	187	C7H3Cl2NO	10
11.	Pyrimidine, 4-(2-hydroxy-5-methoxyphenyl	202	C11H10N2O2	10
12.	2-Amino-4-phenylpyrimidin-1-oxide	187	C10H9N3O	10
13.	Spirohexan-5-one	96	C6H8O	10
14.	Disiloxane, 1,3-dichloro-1,1,3,3-tetrame	202	C4H12Cl2OSi2	10
15.	3,4-DIMETHYL-5-(4-METHYLPHENYL)ISOXAZOLE	187	C12H13NO	9
16.	2(1H)-Pyridinone, 4-hydroxy-6-phenyl-	187	C11H9NO2	9
17.	2-(METHYLAMINO)-1,4-NAPHTHOQUINONE	187	C11H9NO2	9
18.	Silane, trimethyl(octyloxy)-	202	C11H26OSi	9
19.	N-(P-TOLYL)MALEIMIDE	187	C11H9NO2	9
20.	Benzene, 1-isocyanato-3-(trifluoromethyl	187	C8H4F3NO	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	23	022384-08-3	36883	41	85	2	99	50	6	0	29	7965
2.	12	000690-94-8	2158	38	70	3	99	65	2	5	31	3550
3.	*10	021905-54-4	28521	33	91	2	91	80	1	0	39	7808
4.	*10	016511-39-0	127435	35	85	2	83	72	1	0	39	7880
5.	*10	002285-12-3	28718	60	50	1	68	80	1	14	39	7804
6.	*10	001204-06-4	28816	43	79	2	94	80	1	0	39	7808
7.	*10	039920-37-1	28685	56	61	2	74	70	1	5	34	8144
8.	*10	041195-90-8	28689	51	70	3	85	70	1	12	37	8125
9.	*10	000000-00-0	28732	33	65	1	80	79	1	11	40	7910
10.	*10	005392-82-5	28684	47	66	2	99	71	1	13	38	8062
11.	10	097630-77-8	35506	44	59	1	82	80	1	0	39	7835
12.	*10	080830-43-9	28787	43	64	2	67	80	1	5	40	7808
13.	*10	020061-22-7	598	32	79	2	69	65	1	0	29	3645
14.	10	002401-73-2	128464	47	77	3	95	80	1	14	38	7843
15.	* 9	061314-43-0	28854	44	60	3	98	78	1	7	30	7525
16.	* 9	017424-17-8	28814	33	77	2	77	76	1	5	32	7832
17.	* 9	014423-00-8	28830	41	66	2	85	80	1	8	34	7808
18.	9	014246-16-3	128517	46	73	1	67	80	1	0	34	7802
19.	* 9	001631-28-3	28813	40	63	2	96	80	1	7	37	7837
20.	* 9	000329-01-1	28719	42	77	2	99	80	1	0	33	7804

Peak 62 (Coeluting compounds)



Scan 933 (20.469 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.80	841	60.90	292	75.05	300	90.00	50
47.80	110	62.00	392	75.95	106	91.00	2797
48.95	263	62.95	44	77.05	2283	91.95	673
49.95	452	63.95	169	78.05	789	93.05	7676
50.95	1214	65.00	1507	79.05	1734	94.05	666
52.00	176	66.00	204	80.00	199	96.00	56
53.05	1888	67.05	892	81.00	560	97.00	93
55.05	263	67.95	282	83.00	62	101.00	17
55.90	1	69.00	836	83.95	121	102.05	967
57.00	58	69.95	14	87.00	359	103.00	20
59.90	60	72.05	126	89.00	621	105.00	399

Scan 933 (20.469 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	1198	129.00	3275	143.05	230	170.95	300
108.00	71	129.90	528	143.95	1045	171.95	330
109.00	557	131.00	1476	145.05	407	181.90	53
115.00	817	132.00	137	146.00	160	190.95	98
116.10	71	133.00	245	146.95	64	191.95	50
117.05	580	134.15	410	151.15	1	205.90	171
118.00	2	135.00	3472	153.00	26		
119.05	1396	136.10	443	155.00	317		
123.05	215	137.00	402	156.90	106		
126.00	146	138.00	165	159.00	131		
127.05	660	140.95	226	170.05	1093		

Contains at least three compounds: a terpene (m/z 135, 93 etc); a chlorinated hydrocarbon (m/z 129-131); and a sulpher containing compound (m/z 170-172).

Compounds from Proctor and Gamble A0331.D

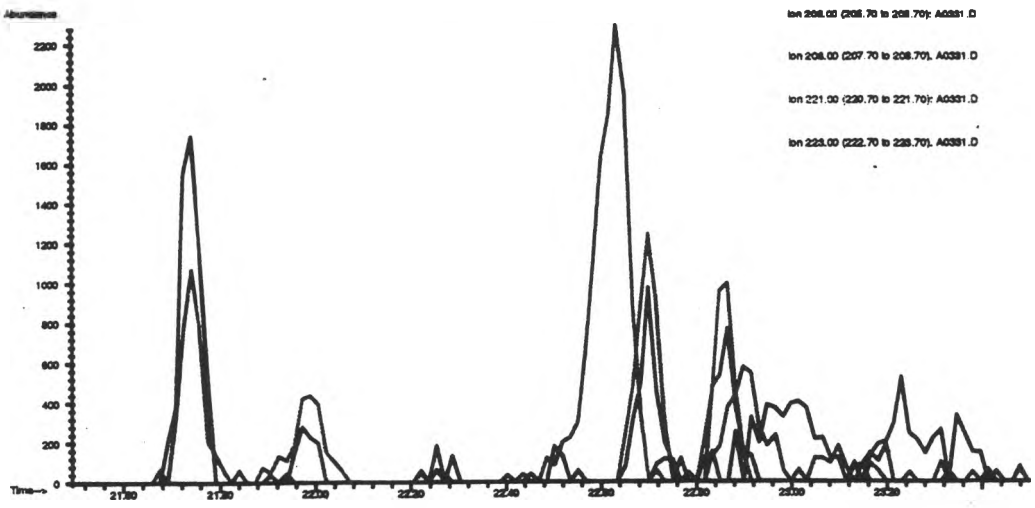
Scan 933 (20.469 min): A0331.D

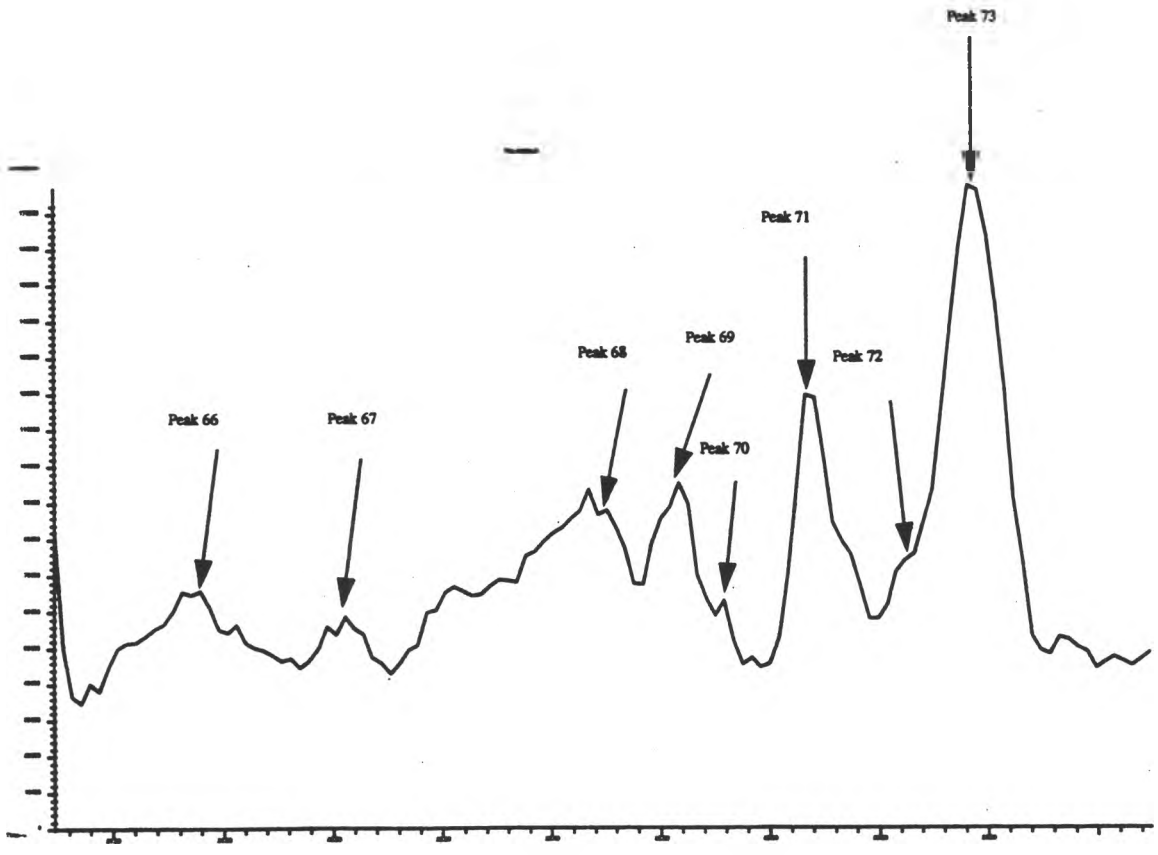
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Pyridine, 2-butyl-	135	C9H13N	43
2.	Acetamide, N-phenyl-	135	C8H9NO	38
3.	.alpha.-Thujene	136	C10H16	22
4.	.alpha.-Thujene	136	C10H16	22
5.	.gamma.-Terpinene	136	C10H16	22
6.	Bicyclo[3.1.0]hexane, 4-methyl-1-(1-meth	136	C10H16	22
7.	cis-Ocimene	136	C10H16	22
8.	1-Phellandrene	136	C10H16	22
9.	Sabinene	136	C10H16	22
10.	THUJENE	136	C10H16	22
11.	BIS[BICYCLO[3.2.0]HEPT-2-EN-4-YL]ETHER	202	C14H18O	22
12.	5,6-DIMETHYL-1,3-CYCLOHEXADIENE	108	C8H12	22
13.	.beta.-Phellandrene	136	C10H16	22
14.	.beta.-Myrcene	136	C10H16	22
15.	Sabinene	136	C10H16	22
16.	.beta.-Myrcene	136	C10H16	22
17.	.beta.-Myrcene	136	C10H16	22
18.	1-Phellandrene	136	C10H16	22
19.	1-Phellandrene	136	C10H16	16
20.	.gamma.-Terpinene	136	C10H16	16

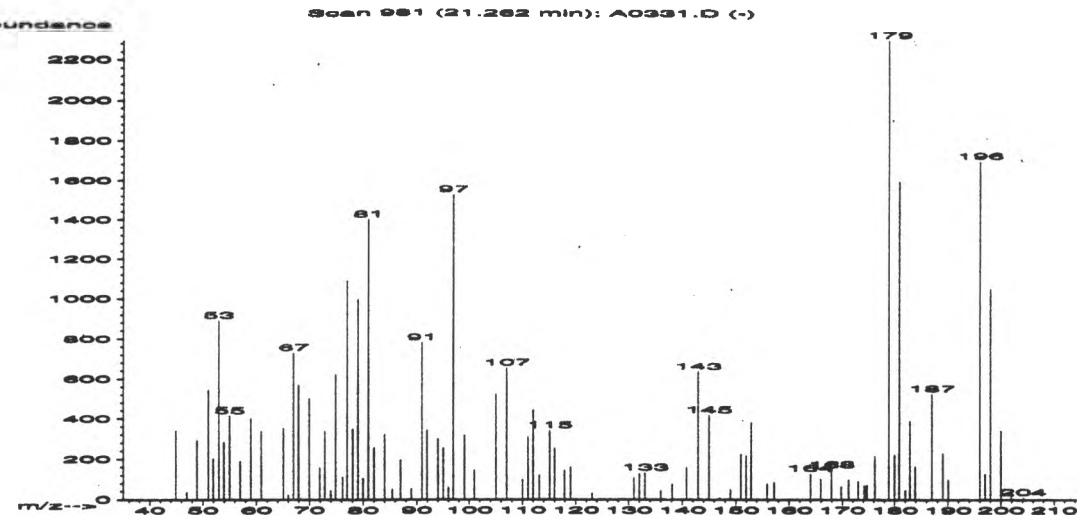
	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	005058-19-5	121727	60	35	1	70	48	18	10	45	8846
2.	*38	000103-84-4	121706	46	42	3	99	48	14	3	38	8848
3.	*22	002867-05-2	122057	34	31	1	74	65	5	1	40	8064
4.	*22	002867-05-2	122055	37	49	1	71	65	5	0	39	8064
5.	22	000099-85-4	122008	46	45	1	87	61	5	4	38	8099
6.	*22	058037-87-9	8157	44	48	1	78	64	5	0	40	8079
7.	*22	029714-87-2	8061	34	73	3	98	63	5	0	39	8131
8.	*22	000099-83-2	121989	35	51	2	99	65	5	20	40	8064
9.	*22	003387-41-5	122063	50	43	1	68	65	5	2	39	8082
10.	*22	002867-05-2	8156	44	48	1	78	64	5	0	40	8079
11.	22	000000-00-0	35758	44	54	2	99	64	5	0	39	8085
12.	22	002417-81-4	1967	43	46	0	78	64	5	0	39	8106
13.	*22	000555-10-2	8118	34	52	1	73	65	5	19	40	8080
14.	*22	000123-35-3	121974	33	67	3	91	64	5	0	41	8093
15.	*22	003387-41-5	122062	50	41	1	81	64	5	18	40	8094
16.	*22	000123-35-3	8068	33	69	2	93	64	5	0	39	8107
17.	*22	000123-35-3	121973	33	67	3	96	65	5	0	41	8064
18.	22	000099-83-2	121990	38	54	2	81	64	5	17	39	8094
19.	16	000099-83-2	121994	45	53	3	99	59	3	0	37	8230
20.	16	000099-85-4	122007	45	49	1	83	59	3	13	37	8169

Compounds from Proctor and Gamble A0331.D





Peak 63



Scan 981 (21.262 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.90	339	65.05	352	78.05	347	94.00	301
46.95	37	66.00	21	79.05	998	95.05	253
48.90	293	67.05	727	80.00	105	96.00	60
51.00	542	67.95	568	81.00	1399	96.95	1521
51.95	203	69.95	500	82.00	256	99.05	316
53.00	890	71.95	158	84.00	322	100.95	145
53.95	281	72.95	338	85.50	49	105.00	521
55.05	414	74.00	43	87.00	196	107.00	654
56.95	189	74.95	620	89.00	52	110.00	99
58.95	401	76.20	111	91.00	781	111.00	307
60.90	338	77.05	1089	91.95	343	112.00	442

Scan 981 (21.262 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
113.15	121	140.80	155	164.00	128	180.00	221
115.05	340	142.95	634	165.95	102	180.90	1592
116.00	251	144.95	417	167.95	147	182.00	45
117.85	141	146.95	8	169.80	63	182.90	390
119.00	161	148.05	1	171.20	99	183.90	163
123.05	30	149.00	49	173.05	92	187.00	526
130.95	107	150.95	224	174.20	69	189.00	229
132.00	129	151.95	217	174.70	72	190.05	98
133.05	131	152.90	381	176.20	216	195.95	1695
136.00	41	155.90	79	177.00	4	196.95	127
138.10	77	157.25	87	178.90	2294	197.95	1054

Scan 981 (21.262 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
199.95	341						
201.90	41						
204.15	10						

Scan 981 (21.262 min): A0331.D

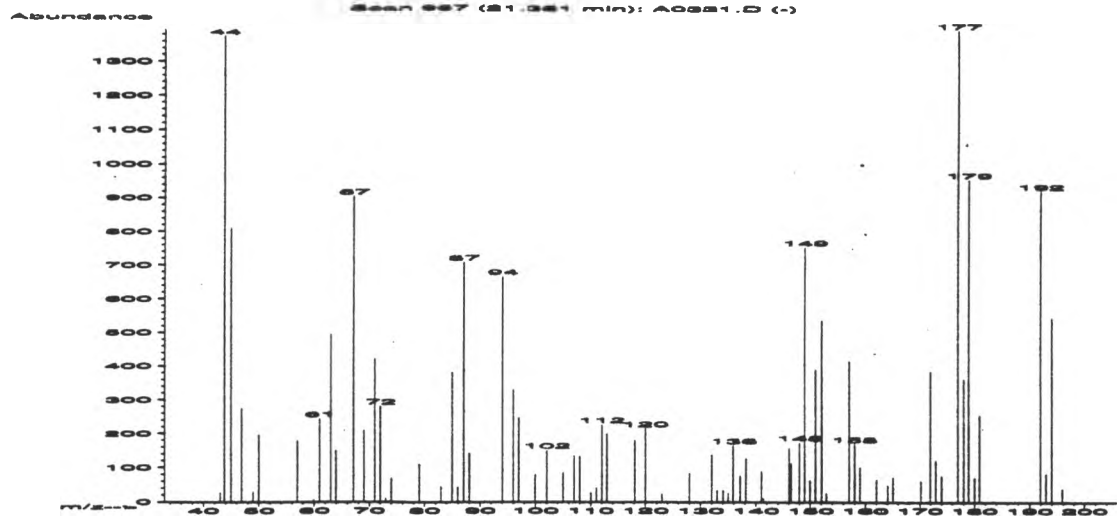
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2,3-.MU.-DIMETHYLCHLOROSILYL-CC'-DIMETHY	196	C6H17B4ClSi	64
2.	Germacyclopent-3-ene, 1,1-dichloro-3-met	212	C5H8Cl2Ge	25
3.	2-Octyne	110	C8H14	14
4.	2-(2,2-Dichloro-1-fluorovinyl)thiophene	196	C6H3Cl2FS	14
5.	1-(.alpha.-Hydroxyacetyl)-2-methylcycloh	196	C11H20OSi	12
6.	METHYL ESTER OF METHYLENE-CYCLOPROPANECA	112	C6H8O2	12
7.	2'-DEOXYCYTIDINIUMCHLORIDE	263	C9H14ClN3O4	12
8.	BENZO(H)ISOQUINOLINE	179	C13H9N	10
9.	N-METHYL-PHENYL-URETHANE	179	C10H13NO2	10
10.	2-BIPHENYLYL VINYL ETHER	196	C14H12O	10
11.	Phenol, 2,4,5-trichloro-	196	C6H3Cl3O	10
12.	DIETHYL 5,6-DIHYDRO-.ALPHA.-PYRAN-6,6-DI	346	C22H34O3	10
13.	N,N-DIETHYL-2,4-PENTADIENEOIC ACID AMIDE	153	C9H15NO	10
14.	.alpha.-Humulene	204	C15H24	10
15.	Benzene, 1,1'-methylenebis[3-methyl-	196	C15H16	10
16.	HISTIDINE THIOHYDANTOIN	196	C7H8N4OS	10
17.	3-ETHYLCYCLOPENT-2-EN-1-ONE	110	C7H10O	10
18.	Naphthalene, 2,3-dichloro-	196	C10H6Cl2	10
19.	2-Octyne	110	C8H14	10
20.	R-7-ENDO-P-PHENYLBENZOYLOXY-6-ANTI-(2'-B	364	C23H24O4	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	036672-04-5	32560	49	96	1	82	7	37	9	34	7821
2.	25	005764-77-2	40012	43	106	1	85	55	7	0	35	4977
3.	*14	002809-67-8	2217	46	73	3	60	69	2	0	39	2212
4.	*14	058229-04-2	32528	33	48	0	66	66	2	0	41	4955
5.	*12	000000-00-0	32901	42	48	2	69	65	2	0	35	5835
6.	*12	000000-00-0	2458	33	78	1	36	63	2	0	35	3698
7.	12	000000-00-0	60700	38	102	0	88	65	2	0	33	4269
8.	*10	000229-71-0	25210	42	57	0	66	77	1	0	39	5743
9.	*10	000000-00-0	126701	46	73	1	71	80	1	0	40	5935
10.	*10	000000-00-0	33159	36	95	2	56	79	1	0	39	6317
11.	*10	000095-95-4	127930	34	91	1	47	80	1	0	39	5724
12.	10	000000-00-0	87124	51	114	2	60	68	1	0	31	2570
13.	*10	000000-00-0	14066	39	60	1	60	69	1	0	33	2212
14.	10	006753-98-6	128670	53	83	1	63	67	1	0	32	2630
15.	*10	021895-14-7	33207	33	105	2	69	75	1	0	39	6266
16.	*10	061160-06-3	32567	33	91	3	127	80	1	0	39	5195
17.	10	000000-00-0	2186	42	55	0	46	69	1	0	33	2212
18.	*10	002050-75-1	32645	33	94	2	70	76	1	0	39	4959
19.	10	002809-67-8	118876	47	56	1	45	69	1	0	34	2212
20.	9	000000-00-0	91239	43	67	1	54	77	1	0	37	4743

Compounds from Proctor and Gamble A0331.D

Peak 64



Scan 987 (21.361 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	25	63.95	150	87.00	707	111.00	40
43.80	1374	67.15	903	88.00	142	112.00	227
44.95	809	69.00	210	94.05	664	112.95	199
46.90	273	70.95	421	95.95	329	118.05	179
48.95	28	72.00	281	96.95	246	119.95	214
49.95	196	72.95	10	99.95	79	122.95	22
50.95	1	74.00	68	102.05	151	128.00	83
56.95	178	79.05	110	105.00	85	132.00	137
59.90	6	83.00	45	107.00	135	133.00	33
61.00	243	85.00	381	108.00	133	134.10	33
63.00	493	85.95	43	110.00	26	135.00	25

Scan 987 (21.361 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
135.90	165	152.95	24	176.95	1394		
137.15	76	157.00	415	178.00	362		
138.15	126	158.00	169	178.90	955		
141.00	89	159.00	100	180.00	72		
146.05	156	162.00	65	180.90	253		
146.45	112	164.05	48	191.95	923		
147.95	173	165.05	72	192.95	83		
148.95	753	170.20	61	194.00	543		
149.95	62	171.95	384	195.85	38		
150.95	389	172.95	120				
152.05	536	174.00	76				

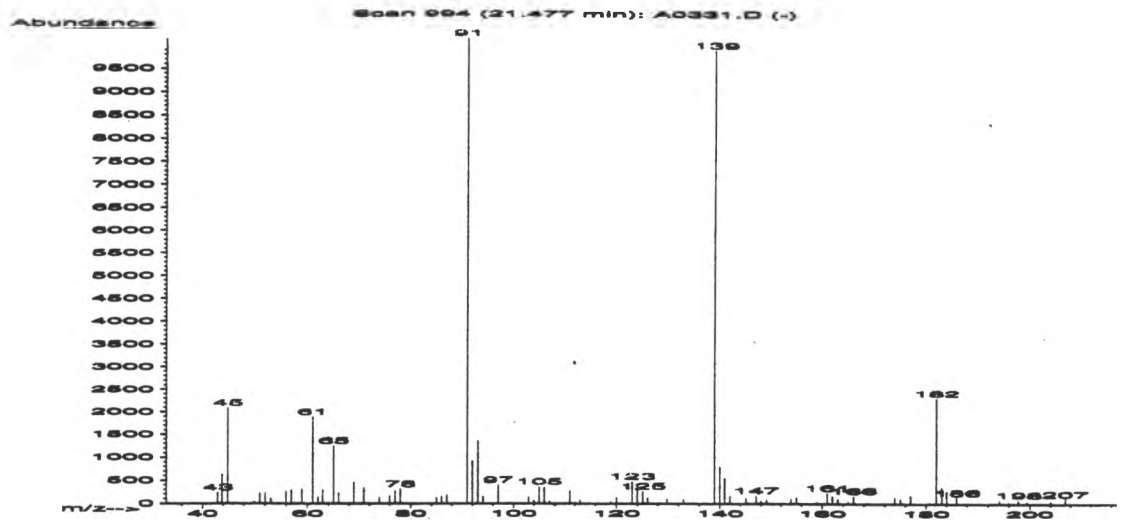
Scan 987 (21.361 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 4,5-dichloro-2-methoxy-	192	C7H6Cl2O2	64
2.	1,4-Benzenediamine, N,N,N'-triethyl-	192	C12H20N2	14
3.	1,4-Benzenediamine, N,N,N'-triethyl-	192	C12H20N2	14
4.	4H-1-Benzopyran-4-one, 2,3-dihydro-7-hyd	192	C11H12O3	14
5.	5-Methyl-4-nitro-2,1-benzisothiazole	194	C8H6N2O2S	14
6.	Phenol, 4-amino-3,5-dichloro-	177	C6H5Cl2NO	14
7.	1-METHOXY-4-CHLORO-NAPHTHALENE	192	C11H9ClO	12
8.	1,4-Benzenediamine, N,N'-bis(1-methyleth	192	C12H20N2	12
9.	(+-)-3,3-Dimethyltricyclo[5.4.0.0(2,9)]u	192	C13H20O	10
10.	1,1,1-Trimethoxytrimethyldisilane	194	C6H18O3Si2	10
11.	9H-Fluorene, 2,3-dimethyl-	194	C15H14	10
12.	ORTHO-XYLENOL-MONOTMS	194	C11H18OSi	9
13.	Isothiazole, 5-bromo-3-methyl-	177	C4H4BrNS	9
14.	5-SEC-BUTYL-4-METHOXY-M-PHENYLENEDIAMINE	194	C11H18N2O	9
15.	Silane, (2,4-dimethylphenoxy)trimethyl-	194	C11H18OSi	9
16.	4(1H)-Pteridinone, 2-amino-7-methyl-	177	C7H7N5O	9
17.	4(1H)-Pteridinone, 2-amino-6-methyl-	177	C7H7N5O	9
18.	Silane, (dimethylphenoxy)trimethyl-	194	C11H18OSi	9
19.	6,7-DIMETHOXY-M-CYMENE	194	C12H18O2	9
20.	4H-1-Benzopyran-4-one, 2,3-dihydro-7-hyd	192	C11H12O3	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	002460-49-3	30514	84	41	1	81	50	37	39	90	8101
2.	*14	024340-91-8	127714	35	112	2	93	68	2	0	39	6810
3.	*14	024340-91-8	30927	35	112	2	92	68	2	0	39	6810
4.	*14	017771-33-4	30751	37	92	2	99	67	2	0	39	6853
5.	*14	074960-03-5	31508	41	79	0	45	69	2	0	39	6439
6.	*14	026271-75-0	24095	35	76	0	99	70	2	0	41	6883
7.	*12	010443-43-3	30705	30	77	0	45	65	2	14	35	7995
8.	12	004251-01-8	30928	39	70	1	77	63	2	5	31	7303
9.	*10	057768-52-2	31072	36	120	3	66	75	1	0	39	6203
10.	*10	018000-25-4	31446	37	61	1	54	68	1	8	37	4232
11.	*10	004612-63-9	127891	37	68	1	46	76	1	0	39	5026
12.	* 9	000000-00-0	31806	39	82	1	52	76	1	0	35	5306
13.	* 9	020493-60-1	24090	35	83	3	75	80	1	0	30	6758
14.	* 9	000000-00-0	31797	36	71	2	68	79	1	0	35	4538
15.	* 9	016414-81-6	31808	37	73	1	66	76	1	8	37	4909
16.	* 9	013040-58-9	24107	34	74	2	90	79	1	0	35	5792
17.	* 9	000708-75-8	24106	33	70	2	67	78	1	0	35	5903
18.	* 9	072088-22-3	31813	39	82	1	52	76	1	0	35	5306
19.	* 9	000000-00-0	31876	40	80	2	68	78	1	8	37	4771
20.	* 8	017771-33-4	127697	32	96	3	82	70	1	0	29	6807

Peak 65



Scan 994 (21.477 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	236	62.00	138	86.00	157	107.00	49
43.80	636	62.95	295	87.00	188	108.00	4
44.95	2083	65.00	1244	91.00	10138	111.00	274
49.95	41	66.00	214	92.00	921	112.05	24
51.00	214	68.95	459	93.05	1351	113.00	64
52.00	226	70.95	331	94.05	143	118.95	37
53.05	109	73.95	118	96.95	402	120.00	125
56.00	255	75.95	168	103.00	141	123.00	475
57.00	291	77.05	262	104.00	59	124.00	349
58.95	306	78.05	306	105.00	366	125.05	260
61.00	1877	85.00	122	106.00	342	126.00	115

Scan 994 (21.477 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
129.75	99	155.00	121	180.85	16		
133.00	90	159.10	37	182.00	2304		
139.00	9881	161.00	225	183.10	339		
140.00	777	162.00	150	184.00	256		
140.95	549	163.00	94	186.00	124		
141.95	160	164.95	56	194.20	66		
145.05	110	166.00	163	195.90	43		
147.05	165	168.85	23	197.80	77		
148.00	55	173.95	125	199.45	38		
149.10	75	175.05	93	204.10	61		
153.95	94	176.95	167	207.00	100		

Compounds from Proctor and Gamble A0331.D

Scan 994 (21.477 min): A0331.D

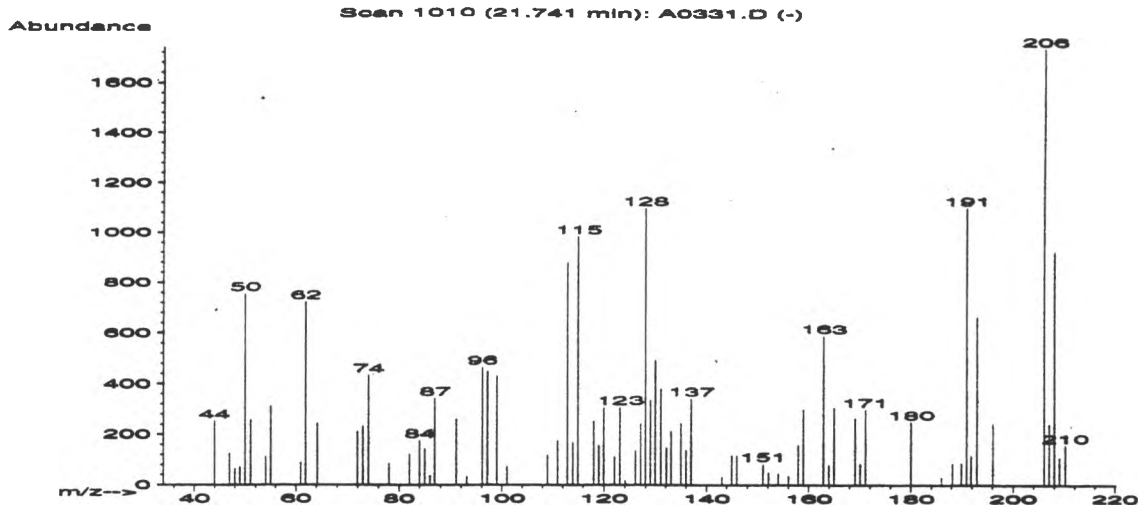
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Thiophene, 2-isobutyl-5-propyl-	182	C11H18S	52
2.	1-Propanone, 1-(3-chlorophenyl)-2-methyl	182	C10H11ClO	47
3.	2(1H)-Pyridinethione, 1,6-dimethyl-	139	C7H9NS	47
4.	Thiophene, 2-butyl-5-propyl-	182	C11H18S	40
5.	Benzene, chloro(1-methylbutyl)-	182	C11H15Cl	38
6.	5-Hydroxymethylthiophen-3-carbonitrile	139	C6H5NOS	38
7.	2(1H)-Pyridinethione, 1,5-dimethyl-	139	C7H9NS	38
8.	2(1H)-Pyridinethione, 1,3-dimethyl-	139	C7H9NS	38
9.	Phenol, 2-nitro-	139	C6H5NO3	38
10.	Phenol, 2-nitro-	139	C6H5NO3	38
11.	2(1H)-Pyridinethione, 1,4-dimethyl-	139	C7H9NS	37
12.	Benzenamine, N-sulfinyl-	139	C6H5NOS	33
13.	DIPHENYL ETHANE	182	C14H14	25
14.	N-PROPYL-P-TOLUENESULFINAMIDE	197	C10H15NOS	25
15.	Pyridine, 4-(ethylthio)-	139	C7H9NS	23
16.	Benzene, 1,1'-(1,2-ethanediyl)bis-	182	C14H14	18
17.	Benzene, 1,1'-(1,2-ethanediyl)bis-	182	C14H14	14
18.	1-METHYL-4,5-DIETHYL-4-IMIDAZOLIN-2-ONE	154	C8H14N2O	14
19.	Acetic acid, [(phenylmethyl)thio]-	182	C9H10O2S	12
20.	Benzene, 1,1'-(1,2-ethanediyl)bis-	182	C14H14	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*52	004861-63-6	26736	50	56	3	84	35	27	0	46	6943
2.	*47	055649-98-4	26462	33	58	3	90	40	20	6	39	6696
3.	*47	019006-69-0	8904	47	48	1	67	40	20	0	40	6848
4.	*40	004861-62-5	26735	40	75	2	75	34	16	0	33	7036
5.	*38	054657-99-7	26597	29	91	3	72	40	14	0	33	6716
6.	*38	080577-96-4	8851	28	47	0	73	37	14	8	35	6886
7.	*38	019006-68-9	8903	34	67	2	75	40	14	0	35	6863
8.	*38	019006-66-7	8901	42	56	1	68	40	14	0	33	6865
9.	*38	000088-75-5	122359	34	50	2	89	50	14	14	39	6780
10.	*38	000088-75-5	122358	33	45	0	66	50	14	9	39	6781
11.	*37	019006-67-8	8902	39	61	1	72	42	13	0	33	6789
12.	*33	001122-83-4	122355	28	55	3	93	34	10	0	27	8346
13.	*25	000000-00-0	127065	33	37	2	92	65	7	2	43	7108
14.	25	006873-85-4	33321	33	57	2	69	42	7	0	22	7490
15.	*23	013669-34-6	122376	26	41	1	73	48	6	1	23	6807
16.	*18	000103-29-7	127068	53	32	1	75	70	3	0	49	7111
17.	*14	000103-29-7	127070	45	44	3	92	67	2	0	40	7110
18.	*14	059167-89-4	14345	32	47	0	53	70	2	13	42	6752
19.	*12	000103-46-8	126975	36	63	3	99	64	2	0	30	7246
20.	*11	000103-29-7	26887	49	37	1	81	71	2	0	46	7110

Compounds from Proctor and Gamble A0331.D

Peak 66 (Dichloroveratrole)



Scan 1010 (21.741 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	252	71.95	210	96.05	465	119.95	306
46.90	125	73.00	232	97.05	449	122.05	112
47.95	63	74.05	434	99.00	429	123.05	308
48.95	71	78.05	85	101.00	73	124.05	16
49.95	754	82.00	124	109.00	119	126.00	137
51.00	257	84.00	176	111.00	178	127.05	243
54.00	113	85.00	143	112.90	882	127.95	1099
55.05	312	86.00	36	114.00	170	129.00	334
60.95	90	86.90	344	115.00	986	129.90	493
61.90	722	91.00	261	118.05	254	131.00	379
64.15	243	93.05	33	119.00	157	132.15	147

Scan 1010 (21.741 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.00	213	158.00	160	189.95	89		
134.95	245	159.00	300	190.95	1102		
136.00	138	162.90	591	191.85	117		
137.00	342	163.95	80	192.95	667		
143.00	32	164.95	308	196.05	245		
144.95	118	169.05	266	206.00	1739		
145.95	116	170.05	85	207.00	243		
151.05	84	171.05	300	208.00	929		
152.10	49	180.00	251	209.00	110		
154.00	46	186.00	32	210.15	160		
156.00	37	188.15	87				

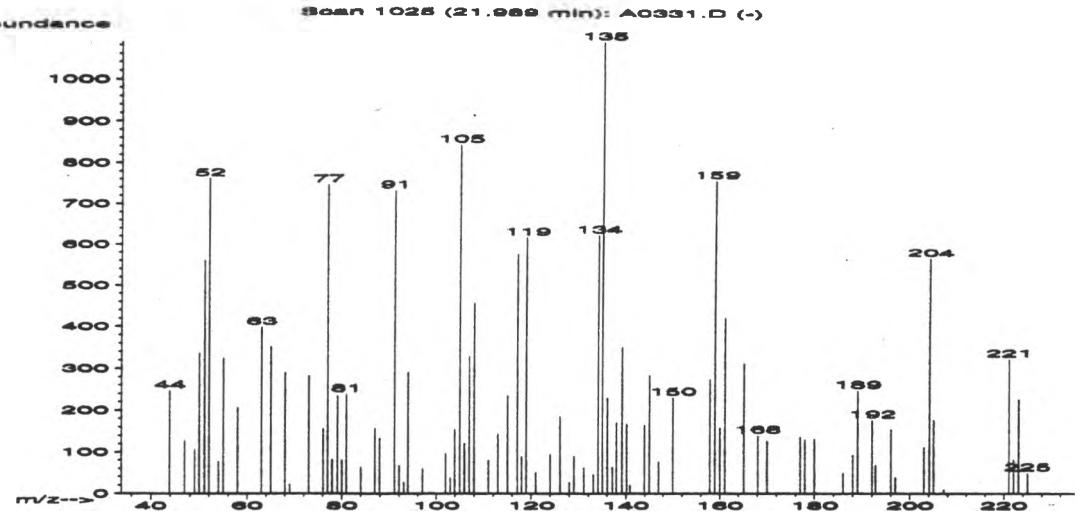
Scan 1010 (21.741 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	trans-3,5-Dichloro-2-fluoro-2,3-dihydrob	206	C8H5Cl2FO	83
2.	cis-3,5-Dichloro-2-fluoro-2,3-dihydroben	206	C8H5Cl2FO	83
3.	cis-2,5-Dichloro-3-fluoro-2,3-dihydroben	206	C8H5Cl2FO	83
4.	trans-2,5-Dichloro-3-fluoro-2,3-dihydrob	206	C8H5Cl2FO	83
5.	Benzene, 1,4-dichloro-2,5-dimethoxy-	206	C8H8Cl2O2	62
6.	1,3-Dichloro-4,6-dimethoxybenzene	206	C8H8Cl2O2	52
7.	Benzo[b]thiophen-3(2H)-one, 2-diazo-, 1,	208	C8H4N2O3S	37
8.	6,7-Dimethoxy-5-benzofurancarboxaldehyde	206	C11H10O4	27
9.	Benzenamine, 2,6-dichloro-4-nitro-	206	C6H4Cl2N2O2	27
10.	Benzene, dichlorodimethoxy-	206	C8H8Cl2O2	25
11.	2-(2,6-DIMETHYLPHENYL)IMINO-2-THIAZOLINE	206	C11H14N2S	22
12.	Benzenamine, 2,6-dichloro-4-nitro-	206	C6H4Cl2N2O2	18
13.	Norseychellanone	206	C14H22O	14
14.	Benzenamine, 2,6-dichloro-4-nitro-	206	C6H4Cl2N2O2	14
15.	1,1-Diphenyl-1-butene	208	C16H16	11
16.	2H-1-Benzopyran-2-one, 6,7-dimethoxy-	206	C11H10O4	11
17.	3,6-Dichloro-2-nitro-aniline	206	C6H4Cl2N2O2	11
18.	1,3-BUTADIENE, 1,1-DIPHENYL-	206	C16H14	11
19.	4,6-Dichloro-2-nitro-aniline	206	C6H4Cl2N2O2	11
20.	NICKEL, CYCLOPENTADIENYL-1,2,3-TRIMETHYL	206	C11H16Ni	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	086324-85-8	37090	39	8	0	98	0	50	3	42	6680
2.	*83	086324-93-8	37091	39	8	0	98	0	50	3	42	6680
3.	*83	086324-96-1	37093	39	8	0	98	0	50	3	42	6680
4.	*83	086324-88-1	37092	39	8	0	98	0	50	3	42	6680
5.	*62	002675-77-6	128810	74	46	0	76	30	36	28	59	7785
6.	*52	050375-04-7	37102	53	63	0	68	34	27	0	49	7255
7.	*37	001887-57-6	38130	40	85	1	53	41	13	2	37	4688
8.	*27	076439-49-1	37269	34	60	0	99	59	8	0	41	6978
9.	*27	000099-30-9	128801	42	61	1	75	56	8	13	38	6680
10.	*25	072361-17-2	37100	83	50	0	78	76	7	45	80	7381
11.	*22	025332-05-2	37315	37	89	2	91	65	5	11	40	6870
12.	*18	000099-30-9	128800	53	116	2	76	66	3	0	49	7020
13.	*14	020085-94-3	37730	33	54	0	83	70	2	0	41	6247
14.	*14	000099-30-9	128803	45	124	2	78	66	2	0	40	7059
15.	*11	001726-14-3	129013	57	59	1	53	73	2	0	47	3880
16.	*11	000120-08-1	37281	57	77	1	99	73	2	0	49	6967
17.	*11	000000-00-0	37060	35	36	0	79	79	2	4	43	6680
18.	*11	000000-00-0	37775	50	97	1	68	80	2	0	44	7816
19.	*11	000000-00-0	37061	35	44	0	79	79	2	3	43	6680
20.	*10	000000-00-0	37326	35	64	1	99	80	1	13	40	6643

Peak 67



Scan 1025 (21.989 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.85	247	67.95	290	87.90	134	107.00	328
46.95	129	69.00	22	91.05	729	108.00	456
48.95	106	73.05	283	92.00	68	111.00	79
49.95	336	76.05	156	93.00	27	112.95	143
51.00	560	77.05	744	93.95	291	115.00	234
51.95	761	78.00	82	97.05	59	117.05	574
53.95	77	79.05	235	101.95	96	118.05	88
55.00	324	80.00	80	103.00	37	119.00	615
58.00	206	81.00	238	103.95	154	121.00	50
63.00	398	84.00	63	105.00	838	124.00	94
65.00	352	86.90	157	106.00	121	126.05	184

Scan 1025 (21.989 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
128.00	26	140.90	20	168.90	1	196.95	38
128.95	89	143.95	164	170.05	126	203.00	111
131.00	62	144.95	282	176.95	136	204.15	566
133.00	46	146.95	76	178.00	129	205.00	176
134.00	620	150.00	230	180.00	131	207.15	10
135.00	1087	157.90	273	186.00	49	221.05	323
136.05	229	159.00	753	188.00	92	222.05	80
137.05	63	160.00	157	189.00	246	223.05	226
138.00	170	161.10	420	192.05	176	224.95	49
139.15	349	165.05	311	192.80	68		
140.15	166	168.05	139	195.95	153		

Quantitation on 204 & 221 assume halocarbon

Compounds from Proctor and Gamble A0331.D

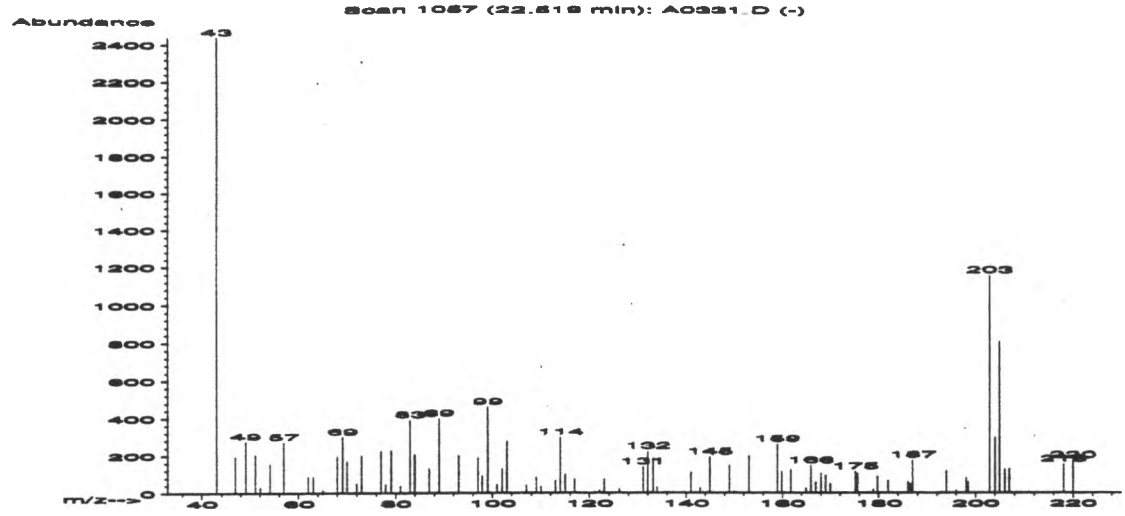
Scan 1025 (21.989 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Valeraldehyde, (o-nitrophenyl)hydrazone	221	C11H15N3O2	27
2.	.alpha.-Patchoulene	204	C15H24	25
3.	Cyclooctatetraene-cyclopentadienyl-chrom	221	C13H13Cr	22
4.	4H-1-Benzopyran-4-one, 2,3-dihydro-6-met	204	C13H16O2	22
5.	Ethanamine, 1-(2,4-cyclopentadien-1-ylid	135	C9H13N	18
6.	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	18
7.	Benzamide, N-methyl-	135	C8H9NO	15
8.	4H-1-Benzopyran-4-one, 2,3-dihydro-6-met	204	C13H16O2	14
9.	1,6-(Chloroisopropylidenyl)-4-methylspir	240	C14H21ClO	14
10.	5-Azidobenzotriazole	160	C6H4N6	14
11.	LONGIBORN-9-ENE	204	C15H24	11
12.	Thiocyanic acid, phenyl ester	135	C7H5NS	11
13.	1H-3a,7-Methanoazulene, octahydro-1,9,9-	204	C15H24	11
14.	METHYL 5-OXO-1,2,4-METHENO-2,3,3A,4,5,7A	204	C12H12O3	10
15.	Benzaldehyde, 4-methyl-, oxime, (Z)-	135	C8H9NO	10
16.	1H-Indene, 2,3,3a,4-tetrahydro-3,3a,6-tr	204	C15H24	10
17.	Cyclopropene, 1,3-dimethyl-2,3-bis(trifl	204	C7H6F6	10
18.	3.ALPHA.-T-BUTYL-1,2,3,4,4A.BETA.,5,6,7-	192	C14H24	10
19.	O-(N-METHYLFORMIMIDOYL)PHENOL	135	C8H9NO	10
20.	Benzene, 1-azido-4-methyl-	133	C7H7N3	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	27	005977-70-8	44202	46	104	3	128	59	8	11	38	5250
2.	*25	000560-32-7	128713	53	106	3	98	64	7	0	47	7519
3.	*22	057002-78-5	129767	45	74	0	66	62	5	14	40	4585
4.	*22	051423-97-3	36514	45	75	1	88	62	5	0	40	7002
5.	*18	014469-77-3	7590	52	60	1	82	69	3	0	46	6683
6.	*18	000501-00-8	7538	45	56	0	78	70	3	0	44	6497
7.	*15	000613-93-4	121708	61	40	0	94	77	2	26	55	6117
8.	*14	051423-98-4	36512	39	78	0	99	66	2	0	39	6770
9.	14	086678-46-8	130805	45	21	0	58	68	2	0	39	4558
10.	*14	000000-00-0	16563	37	42	0	49	69	2	0	41	3780
11.	*11	061262-67-7	36703	45	79	0	50	78	2	0	44	4360
12.	*11	005285-87-0	7525	43	58	0	99	77	2	0	44	5823
13.	*11	000508-55-4	36710	52	101	1	44	74	2	0	44	6674
14.	*10	065055-59-6	36425	33	61	0	39	78	1	0	41	3939
15.	*10	003717-16-6	7569	33	93	1	95	77	1	0	39	6014
16.	*10	059742-39-1	36696	35	115	1	54	74	1	0	39	5526
17.	*10	054932-73-9	36130	50	78	0	85	76	1	2	41	6218
18.	*10	058729-09-2	31117	35	30	1	78	78	1	0	39	5319
19.	*10	000000-00-0	7573	37	65	0	67	77	1	0	41	6036
20.	10	002101-86-2	121456	56	72	3	100	70	1	0	36	3724

Peak 68



Scan 1057 (22.519 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2439	67.95	199	86.95	132	110.00	35
46.85	193	69.05	301	89.00	401	113.00	69
48.95	274	70.05	169	93.05	203	114.00	301
50.95	205	72.00	51	97.05	190	115.00	101
52.05	30	72.95	203	97.95	94	116.95	76
54.05	156	77.00	227	99.05	464	121.05	8
55.95	5	77.95	46	101.00	45	122.05	16
56.90	273	79.05	229	102.05	132	123.00	76
61.95	89	81.00	39	103.00	279	126.05	23
63.00	88	83.00	393	107.00	42	131.00	142
65.00	16	83.90	209	109.00	87	132.00	224

Scan 1057 (22.519 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.05	187	164.95	26	186.00	61	206.00	129
133.95	31	165.95	148	186.40	50	206.90	130
141.00	113	166.95	59	187.00	178	218.05	155
142.95	28	168.00	107	193.00	8	219.95	176
144.95	195	169.00	98	193.95	122		
149.05	148	170.00	50	195.95	16		
150.05	9	175.20	117	198.05	81		
153.10	201	175.55	106	198.45	58		
158.95	263	178.90	19	202.90	1159		
159.90	114	179.75	90	204.00	298		
161.75	126	181.90	68	204.90	809		

Compounds from Proctor and Gamble A0331.D

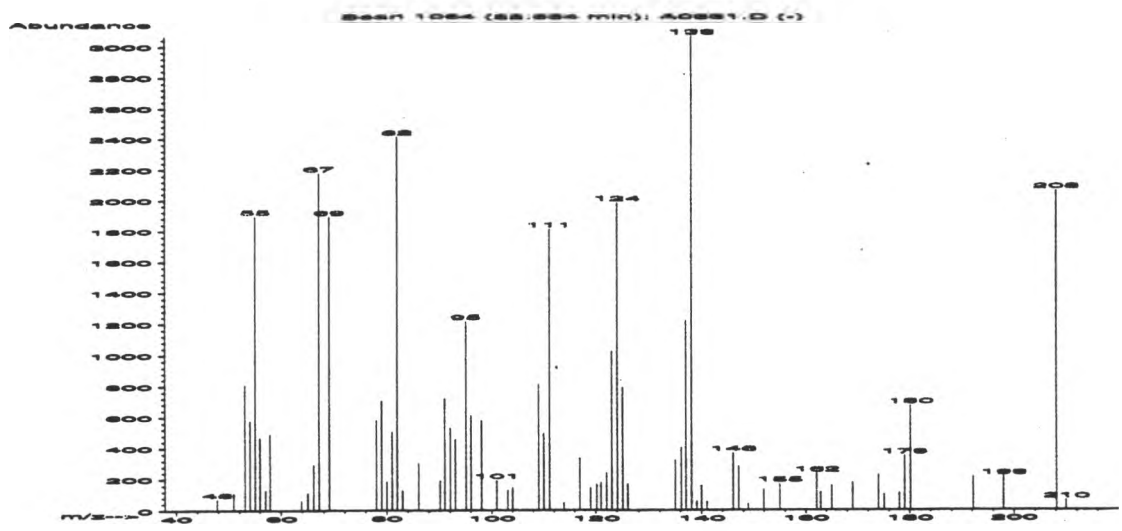
Scan 1057 (22.519 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	ETHYL N-ALLYL-N-PHENYLCARBAMATE	205	C12H15NO2	9
2.	1H-Indole-2-carboxylic acid, 6-hydroxy-,	205	C11H11NO3	7
3.	Propane, 1-chloro-3-iodo-	204	C3H6ClI	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.*	9	000000-00-0	36934	41	99	2	51	78	1	0	35	5347
2.*	7	015050-03-0	36921	28	122	3	73	78	1	0	27	5347
3.*	7	006940-76-7	36083	28	74	1	30	78	1	0	29	2816

Peak 69



Scan 1064 (22.634 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
47.85	72	66.10	297	90.15	192	109.00	815
50.95	109	67.05	2173	91.00	722	110.00	493
51.95	3	69.05	1890	92.05	531	111.10	1810
53.05	810	69.95	4	93.05	460	113.90	49
54.05	577	78.05	582	95.05	1218	116.95	336
55.05	1893	79.05	706	96.05	610	119.00	143
56.00	469	80.00	184	98.05	578	120.20	168
57.00	130	81.00	506	100.95	193	121.00	177
57.90	492	82.00	2403	103.05	129	122.05	241
63.80	61	83.00	128	104.00	146	123.05	1029
65.00	113	86.00	304	106.00	5	124.05	1983

Scan 1064 (22.634 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
125.05	793	148.95	39	180.15	674		
126.00	170	151.95	131	192.20	215		
135.00	324	155.00	169	193.00	5		
136.15	407	162.15	235	198.05	216		
137.00	1224	162.90	118	208.15	2059		
138.15	3063	165.00	161	210.00	64		
139.10	57	169.05	177				
140.00	158	173.95	227				
141.00	55	175.05	101				
146.05	370	178.00	114				
147.05	281	179.00	350				

Compounds from Proctor and Gamble A0331.D

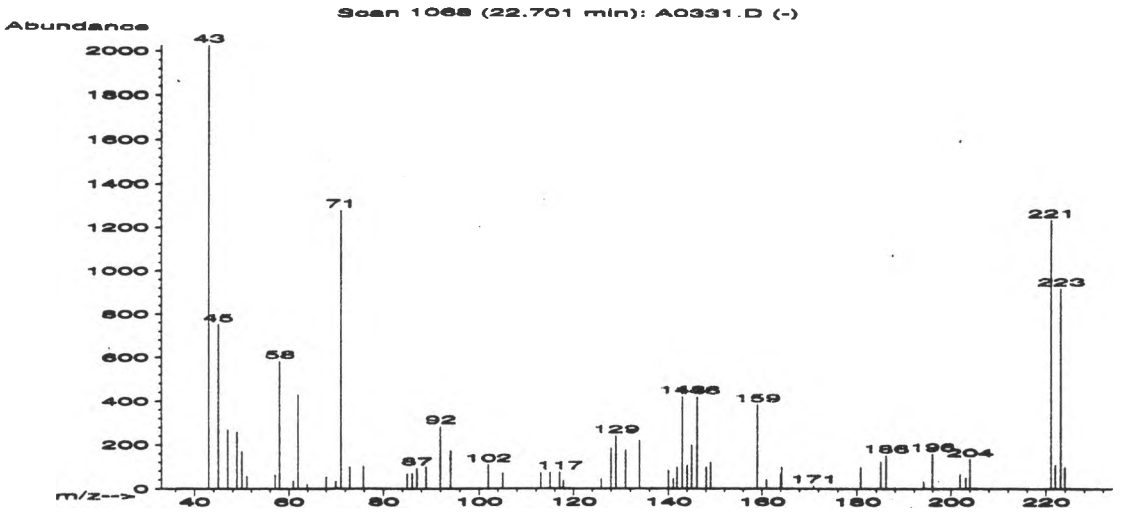
Scan 1064 (22.634 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Naphthalene, decahydro-	138	C10H18	46
2.	Naphthalene, decahydro-, cis-	138	C10H18	38
3.	Naphthalene, decahydro-, trans-	138	C10H18	38
4.	Bicyclo[3.3.1]nonan-9-one	138	C9H14O	27
5.	Naphthalene, decahydro-	138	C10H18	22
6.	Benzene, 1,3-dimethoxy-	138	C8H10O2	18
7.	2H-Benzocyclohepten-2-one, decahydro-9a-	180	C12H20O	15
8.	Naphthalene, decahydro-, cis-	138	C10H18	14
9.	Cyclopropane, 1,1-dimethyl-2-(1-methylet	152	C11H20	14
10.	Naphthalene, decahydro-	138	C10H18	14
11.	2-Adamantanecarboxylic acid, 4,8-dioxo-	208	C11H12O4	11
12.	Acetic acid, mercapto-, cyclohexyl ester	174	C8H14O2S	10
13.	Benzene, 1-methyl-4-(methylthio)-	138	C8H10S	10
14.	D-erythro-Pent-1-enitol, 1,5-anhydro-2-d	154	C7H11BO3	10
15.	Benzene, 1-methyl-4-(methylthio)-	138	C8H10S	10
16.	10,10-DIMETHYL-6-METHYLIDEN-1-OXA-SPIRO(	180	C12H20O	10
17.	2,3,10,10-TETRAMETHYL-6-METHYLEN-1-OXA-S	208	C14H24O	10
18.	2(1H)-Naphthalenone, octahydro-1,4a-dime	180	C12H20O	10
19.	3-Hexyne	82	C6H10	10
20.	2,4-Hexadiene	82	C6H10	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	000091-17-8	122339	66	57	2	70	52	20	0	64	7199
2.	*38	000493-01-6	122334	53	76	3	84	52	14	0	47	7209
3.	*38	000493-02-7	122344	53	72	2	70	52	14	0	47	7195
4.	*27	017931-55-4	122278	54	58	3	87	59	8	17	38	6975
5.	*22	000091-17-8	122335	43	80	2	67	61	5	0	40	7169
6.	*18	000151-10-0	8523	53	54	1	74	70	3	0	47	5932
7.	*15	055103-67-8	25810	59	76	1	59	71	2	0	51	5565
8.	*14	000493-01-6	122337	33	79	3	99	66	2	17	39	7133
9.	14	056701-50-9	13866	47	60	0	66	66	2	19	41	5169
10.	*14	000091-17-8	122340	33	79	3	99	66	2	17	39	7089
11.	*11	005202-69-7	38319	57	85	2	64	78	2	0	49	4778
12.	*10	016849-98-2	22810	33	77	1	125	80	1	0	39	4266
13.	*10	000623-13-2	8558	35	70	3	98	73	1	0	39	5991
14.	10	074793-26-3	124130	55	73	0	57	73	1	0	39	5045
15.	*10	000623-13-2	122250	44	66	3	90	73	1	0	40	6105
16.	*10	043125-87-7	25781	36	78	0	59	79	1	0	41	4830
17.	*10	060745-31-5	128996	46	79	3	167	76	1	0	40	4463
18.	*10	022738-31-4	25796	44	88	1	56	80	1	0	40	3322
19.	*10	000928-49-4	116763	45	62	1	70	80	1	0	39	4266
20.	*10	000592-46-1	116772	33	51	1	60	80	1	11	40	4266

Peak 70



Scan 1068 (22.701 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2027	68.00	54	101.95	109	140.00	84
44.95	751	69.95	34	105.00	70	141.05	45
46.95	268	71.05	1277	113.00	71	141.85	99
48.90	259	72.95	100	115.00	73	142.95	420
49.95	170	75.80	102	117.05	75	144.00	105
51.00	59	85.00	68	117.85	37	144.95	198
57.00	64	86.00	69	125.95	44	146.05	418
58.00	582	87.00	93	127.95	184	148.05	97
60.95	36	89.00	100	129.00	242	149.00	121
61.90	428	91.95	284	131.00	176	159.00	383
63.90	20	94.05	174	133.90	219	161.00	40

Scan 1068 (22.701 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.90	66	204.00	135				
164.15	99	221.05	1238				
171.00	14	221.95	107				
180.80	99	223.05	923				
184.95	123	223.95	98				
186.00	153						
187.95	6						
194.05	34						
195.95	160						
201.90	66						
203.10	49						

Compounds from Proctor and Gamble A0331.D

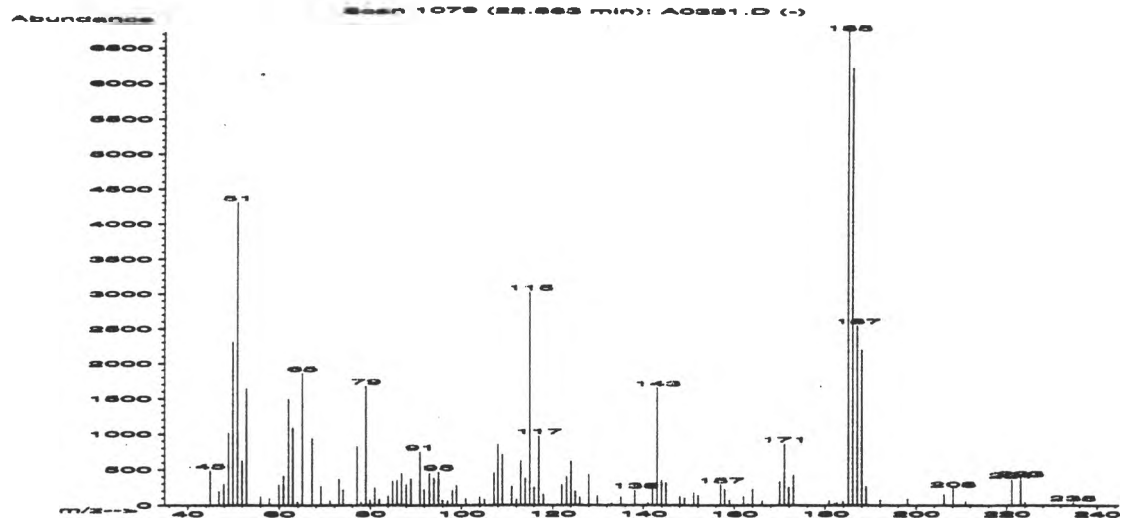
Scan 1068 (22.701 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-Bromo-1-phenylpyrrole	221	C10H8BrN	10
2.	2-(TRIFLUOROMETHYL)-7H-1,3,4-THIADIAZOLO	221	C6H2F3N3OS	10
3.	3-Bromo-1-phenylpyrrole	221	C10H8BrN	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*10	030068-53-2	44164	31	35	1	42	64	1	0	29	7081
2.	*10	094605-13-7	44117	33	68	1	46	80	1	0	39	6378
3.	* 8	077124-02-8	44165	31	45	2	42	66	1	0	29	7081

Peak 71 (Chlorovanillin)



Scan 1079 (22.883 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.95	486	60.95	412	77.05	829	89.00	376
46.90	191	62.00	1495	78.00	39	91.00	750
47.95	301	62.95	1091	79.05	1678	91.95	223
48.95	1012	63.95	43	79.95	69	93.05	449
49.95	2308	65.00	1860	81.00	245	94.05	383
50.95	4307	67.15	936	82.00	86	95.05	466
51.95	625	69.05	262	84.00	129	95.95	69
52.95	1638	71.00	59	85.00	341	96.95	56
56.00	118	73.00	373	86.00	354	98.05	209
57.90	96	73.95	218	87.00	447	99.00	279
59.95	287	74.95	3	88.00	287	100.95	93

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.95	113	116.95	974	133.00	19	152.05	140
105.00	87	117.95	153	135.05	119	157.00	291
107.10	459	119.00	5	138.15	213	157.90	229
108.00	858	121.05	18	140.95	35	159.00	78
109.00	718	122.00	291	141.95	301	162.00	122
111.00	265	123.05	401	142.95	1653	163.00	13
112.00	84	124.05	621	143.95	351	164.00	227
113.00	625	125.00	193	144.95	320	166.05	59
114.00	380	126.00	113	147.95	124	169.95	339
115.00	3035	127.95	434	148.95	105	170.95	860
116.00	251	129.90	130	151.00	172	171.95	257

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
172.95	426	198.05	92				
180.85	65	206.15	153				
181.95	20	208.15	236				
182.50	36	211.00	47				
183.90	55	221.05	364				
185.00	6727	223.05	384				
186.00	6214	224.05	40				
187.00	2559	234.65	38				
188.00	2200						
188.90	266						
192.00	75						

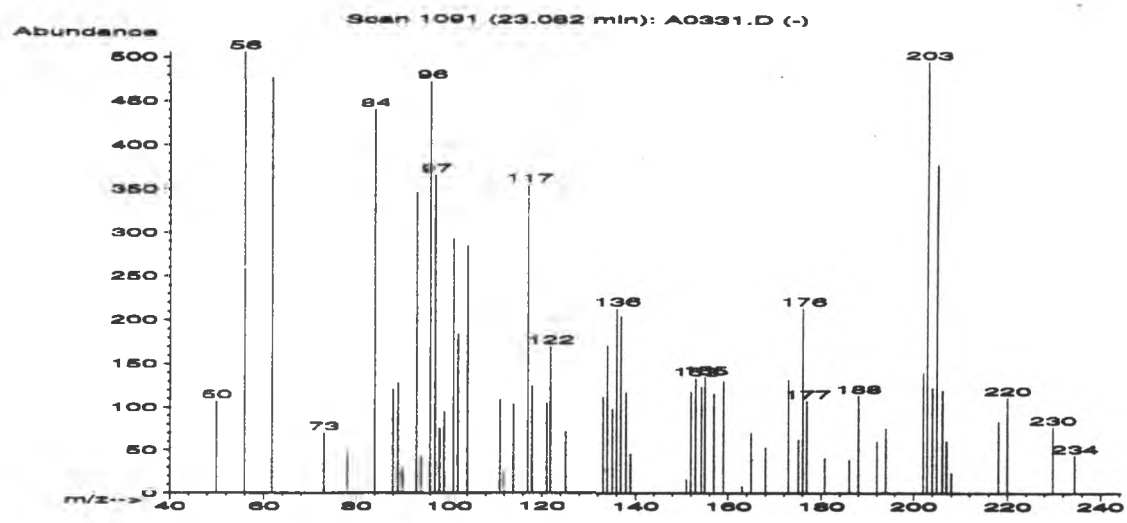
Scan 1079 (22.883 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	E-2-BENZYLIDENE CYCLOHEXANONE	186	C13H14O	53
2.	[1]Benzothieno[2,3-d]pyridazine	186	C10H6N2S	47
3.	1-Naphthalenecarboxaldehyde, 4-methoxy-	186	C12H10O2	46
4.	E-2-BENZYLIDENE CYCLOHEXANONE	186	C13H14O	35
5.	Cyclohexanone, 2-(phenylmethylene)-	186	C13H14O	32
6.	Benzene, 1,1'-thiobis-	186	C12H10S	25
7.	Benzene, 1,1'-thiobis-	186	C12H10S	12
8.	Benzene, 1,1'-thiobis-	186	C12H10S	12
9.	Ferrocene	186	C10H10Fe	10
10.	Ferrocene	186	C10H10Fe	10
11.	Acetic acid, (4-chlorophenoxy)-	186	C8H7ClO3	10
12.	2-AMINO-5,6-DICHLOROBENZONITRILE	186	C7H4Cl2N2	10
13.	N-DEUTERO-2, 3-DIMETHYL-1H-IMIDAZO(1, 2-	185	C11H10DN3	10
14.	2(3H)-Benzothiazolone, 5-chloro-	185	C7H4ClNOS	10
15.	2-Furancarbodithioic acid, propyl ester	186	C8H10OS2	9
16.	METHYL N,N-BIS(2-CHLOROETHYL)PHOSPHORODI	234	C5H13Cl2N2O2P	9
17.	Pyridine, 2-chloro-3,4,5,6-tetrafluoro-	185	C5ClF4N	9
18.	Benzenesulfonyl chloride, 4-nitro-	221	C6H4ClNO4S	9
19.	Cyclohept[f]indene, 1,2,3,5,6,7,8,9-octa	186	C14H18	8
20.	3-BROMO-P-CRESOL	186	C7H7BrO	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	001467-15-8	28589	50	65	2	74	30	28	0	39	8660
2.	*47	000244-92-8	28331	37	80	2	92	38	20	0	41	6737
3.	*46	015971-29-6	28539	54	70	2	99	42	20	0	47	8744
4.	*35	001467-15-8	127417	45	62	1	82	55	11	16	38	8646
5.	*32	005682-83-7	28588	35	89	2	85	50	9	9	32	8740
6.	*25	000139-66-2	127398	38	76	2	92	51	7	0	35	8642
7.	12	000139-66-2	127397	45	68	3	193	62	2	0	34	8411
8.	12	000139-66-2	28541	46	67	3	191	62	2	0	34	8496
9.	*10	000102-54-5	127347	36	66	0	75	76	1	0	41	5838
10.	*10	000102-54-5	28332	35	65	1	92	75	1	0	39	5826
11.	*10	000122-88-3	127329	38	119	3	88	68	1	0	35	6093
12.	*10	000000-00-0	28129	33	76	3	71	77	1	0	39	5669
13.	10	000000-00-0	27997	45	78	0	50	75	1	0	39	8412
14.	*10	020600-44-6	27878	35	96	2	75	72	1	0	39	6828
15.	* 9	027249-80-5	127331	33	83	1	71	77	1	0	35	5840
16.	9	000000-00-0	49592	43	89	2	79	72	1	0	37	6654
17.	* 9	054774-81-1	27867	38	71	2	99	72	1	0	35	6670
18.	9	000098-74-8	129756	45	85	2	92	76	1	0	37	5769
19.	* 8	007140-25-2	28660	32	99	3	91	70	1	0	29	6453
20.	* 7	000000-00-0	28132	30	86	2	79	71	1	0	27	6022

Peak 72



Scan 1091 (23.082 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.95	107	95.95	471	117.95	125	151.05	16
55.90	506	97.05	364	121.05	105	151.95	117
61.75	477	98.00	76	121.80	170	153.00	133
72.95	70	99.00	95	125.05	72	154.25	123
78.00	46	100.95	292	133.10	112	155.00	135
84.00	439	101.95	184	134.00	171	156.90	115
87.90	121	104.00	284	135.10	98	159.00	130
89.00	129	111.00	109	136.00	213	163.05	8
90.00	29	112.00	25	136.95	204	164.95	70
93.05	345	114.00	104	138.00	117	168.00	53
94.00	43	117.05	353	139.00	46	172.95	132

Scan 1091 (23.082 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
175.05	62	205.00	376				
176.05	213	206.15	119				
176.95	107	207.00	60				
180.75	41	208.00	23				
186.00	39	218.05	83				
188.00	113	219.95	111				
192.05	60	229.75	77				
193.95	75	234.40	44				
202.00	140						
202.90	496						
204.00	122						

Compounds from Proctor and Gamble A0331.D

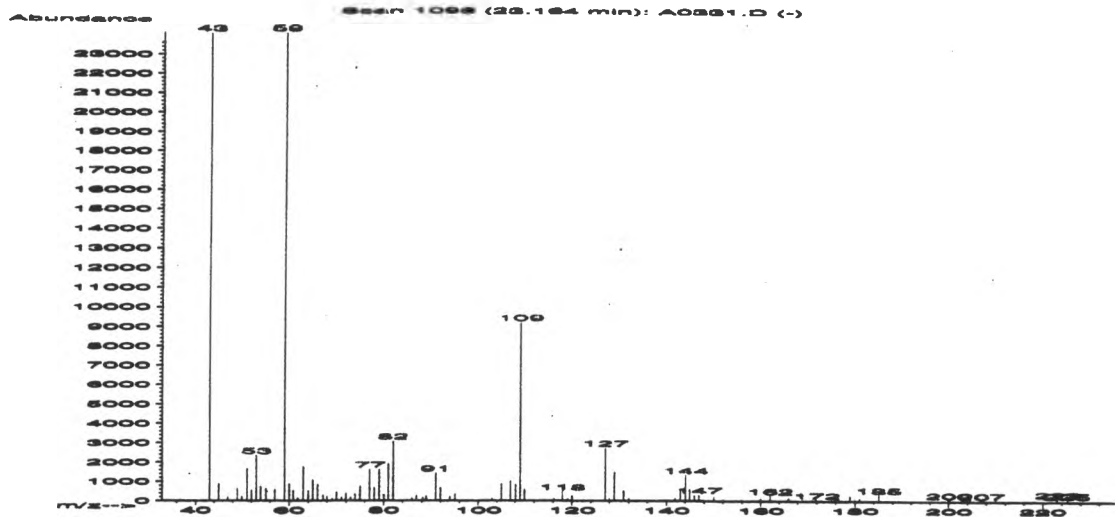
Scan 1091 (23.082 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	6-[18O]-ACETYL-7-HYDROXY-2,2-DIMETHYLBEN	218	C13H14O218O	23
2.	Carbamic acid, tricyclo[2.2.1.0(2,6)]hep	181	C10H15NO2	12
3.	2-(1,1-DIMETHYLETHOXY)-5-(METHYL-D3)THIO	170	C9H11D3OS	12
4.	2,5-DIMETHYL-HEXENE-1-D6	112	C8H10D6	12
5.	6-Hydroxymethylidene-7-isopropylidene-4-	220	C13H16O3	10
6.	4-Amino-5-bromo-6-hydroxy-2-methylpyrimi	203	C5H6BrN3O	10
7.	1-ETHYL[9](2,4)PYRAZOLOPHANE	220	C14H24N2	9
8.	1-AZAPYRENE	203	C15H9N	9
9.	.alpha.-D-Arabinofuranoside, ethyl 2-deo	251	C9H17NO5S	9
10.	2,3-.MU.-TRIMETHYLGERMYL-CC'-DIMETHYL-4,	222	C7H20B4Ge	8
11.	(Z,Z)-5,5'-(2,4-Hexadiendiylidene)bis(1,	206	C16H14	7
12.	2-Bromo-5-dimethylamino-2,4-pentadien-1-	203	C7H10BrNO	7
13.	Benzene, 1-methoxy-2-(1-methylethyl)-, d	218	C10H12Cl2O	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	23	000000-00-0	42816	33	73	2	200	48	6	0	21	5633
2.	12	000709-70-6	26104	33	126	3	234	58	2	0	22	4437
3.	12	054461-03-9	21254	38	89	1	89	58	2	0	28	4437
4.	*12	033718-00-2	2662	28	98	1	99	58	2	0	29	4437
5.	*10	094239-81-3	43669	35	94	1	73	76	1	0	39	3760
6.	10	077708-89-5	35823	35	112	0	56	65	1	0	25	5866
7.	* 9	061936-80-9	43850	32	128	0	61	72	1	0	33	5754
8.	* 9	000000-00-0	36074	31	79	0	98	80	1	0	33	4776
9.	9	056978-64-4	56741	40	132	0	113	74	1	0	33	5661
10.	8	036672-03-4	44401	34	114	1	28	68	1	0	21	5506
11.	7	091524-63-9	37771	34	95	2	74	78	1	0	21	3356
12.	* 7	080487-47-4	35837	30	132	1	71	76	1	0	27	6483
13.	6	074313-04-5	42612	50	113	2	85	78	1	4	19	5610

Peak 73



Scan 1096 (23.164 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	24109	59.00	24123	69.95	456	82.00	3114
44.95	863	60.00	862	71.00	166	86.00	149
46.95	191	60.90	541	71.95	390	86.90	292
48.95	643	61.85	158	73.00	188	88.25	176
49.95	215	63.00	1762	73.95	360	89.00	254
51.00	1673	64.00	512	74.95	792	91.00	1428
52.00	563	65.00	1080	77.05	1630	92.00	683
53.00	2347	66.00	851	78.00	678	93.95	217
53.95	759	67.15	295	79.05	1623	95.05	357
55.05	638	68.00	219	80.00	332	101.95	38
56.95	596	69.05	129	81.00	1931	102.95	119

Scan 1096 (23.164 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.00	886	123.05	8	146.95	315	176.95	31
107.00	1034	127.05	2747	150.05	215	178.90	253
108.05	841	128.00	119	151.95	77	180.00	74
109.00	9236	129.00	1477	156.00	75	181.00	143
110.00	586	131.00	515	160.00	143	185.00	322
115.00	14	132.00	122	162.00	269	200.05	79
116.15	105	141.80	133	165.95	150	202.95	47
117.95	474	142.95	545	170.00	4	204.00	23
119.00	105	144.05	1334	171.00	37	206.20	14
119.95	270	144.95	626	171.95	52	207.00	62
121.90	32	145.95	301	173.00	47	223.05	147

Scan 1096 (23.164 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
225.20	68						

Scan 1096 (23.164 min): A0331.D

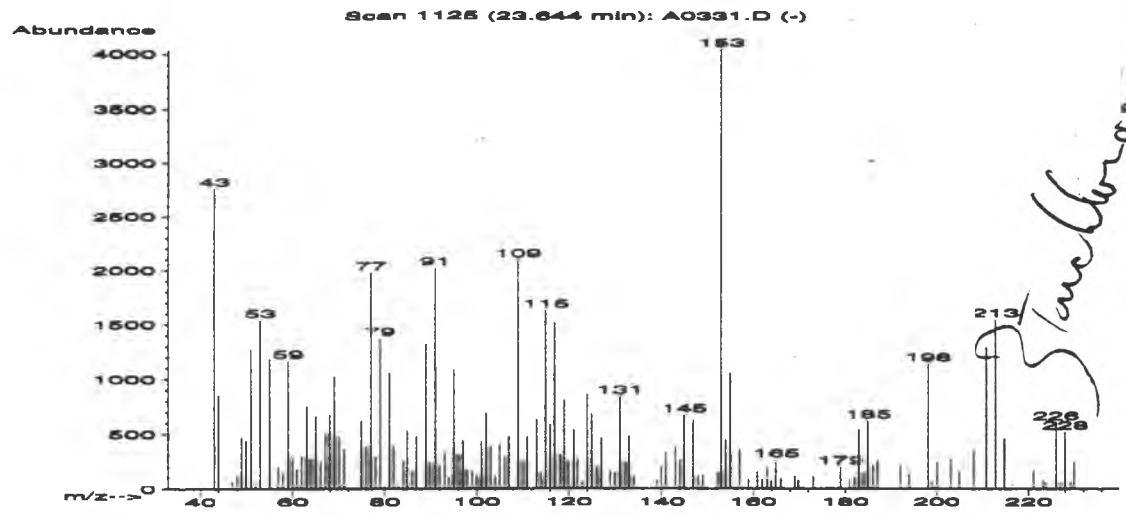
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3-Pentanol	88	C5H12O	32
2.	Silane, (chloromethyl)dimethyl-	108	C3H9ClSi	25
3.	2-Propanone, 1-cyclohexyl-	140	C9H16O	23
4.	Carbonochloridic acid, 1-(chloromethyl)p	170	C5H8Cl2O2	23
5.	Propanoic acid, 2-hydroxy-2-methyl-, eth	132	C6H12O3	23
6.	2-METHOXY-13C-3-METHYLPYRAZINE	124	C513CH8N2O	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*32	000584-02-1	117264	30	47	1	95	50	9	0	33	9177
2.	*25	003144-74-9	1857	28	64	3	99	45	7	0	23	9222
3.	23	000103-78-6	9404	34	60	2	91	50	6	0	22	9237
4.	23	054460-98-9	21053	36	54	2	70	48	6	0	21	9182
5.	23	000080-55-7	6865	36	39	2	92	50	6	0	25	9177
6.	8	034061-82-0	4673	34	144	2	33	69	1	0	21	3527

Compounds from Proctor and Gamble A0331.D

Peak 74



Scan 1125 (23.644 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2762	57.90	147	68.95	1023	83.00	35
43.95	853	59.00	1166	70.05	470	84.00	254
46.95	62	60.00	282	71.05	359	84.95	533
47.95	130	60.95	179	74.95	619	86.00	163
48.95	471	61.95	300	75.95	385	87.00	477
49.95	442	63.00	753	77.00	1977	89.00	1320
50.95	1272	64.00	280	78.05	293	89.90	241
52.00	45	65.00	662	79.00	1371	91.00	2023
53.00	1541	66.00	249	79.95	29	92.00	221
55.05	1185	67.00	512	81.00	1057	93.05	327
56.95	196	67.95	678	82.00	384	93.95	100

Scan 1125 (23.644 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
95.05	1086	106.00	298	118.95	814	131.00	844
96.00	317	107.00	480	119.95	255	132.05	245
97.00	442	109.00	2099	121.05	540	133.00	482
97.95	178	110.00	250	121.95	272	133.95	119
99.00	162	111.00	478	123.00	59	139.05	78
99.95	122	113.00	636	124.05	865	140.00	200
100.95	433	114.00	145	125.00	686	140.95	334
102.05	694	115.00	1635	126.05	202	143.05	378
103.00	382	116.00	589	127.00	468	144.05	261
104.00	119	116.95	1520	128.95	164	144.95	675
105.00	415	118.05	312	129.95	150	146.95	632

Scan 1125 (23.644 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.05	120	163.95	71	183.90	148	208.15	353
149.00	130	164.95	265	184.90	623	210.90	1303
152.15	149	166.05	97	186.00	224	212.90	1560
153.00	4038	169.05	118	187.00	257	214.80	464
154.00	447	169.80	73	192.05	223	216.70	41
155.00	1064	173.05	112	193.95	134	221.05	174
157.00	358	176.95	26	198.05	1142	223.05	74
159.00	82	179.00	198	199.05	62	223.70	54
160.95	160	180.95	88	200.05	244	225.90	614
161.95	85	182.00	101	203.00	275	226.90	51
163.00	195	182.90	546	205.00	163	227.90	528

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
229.15	56						
229.90	244						

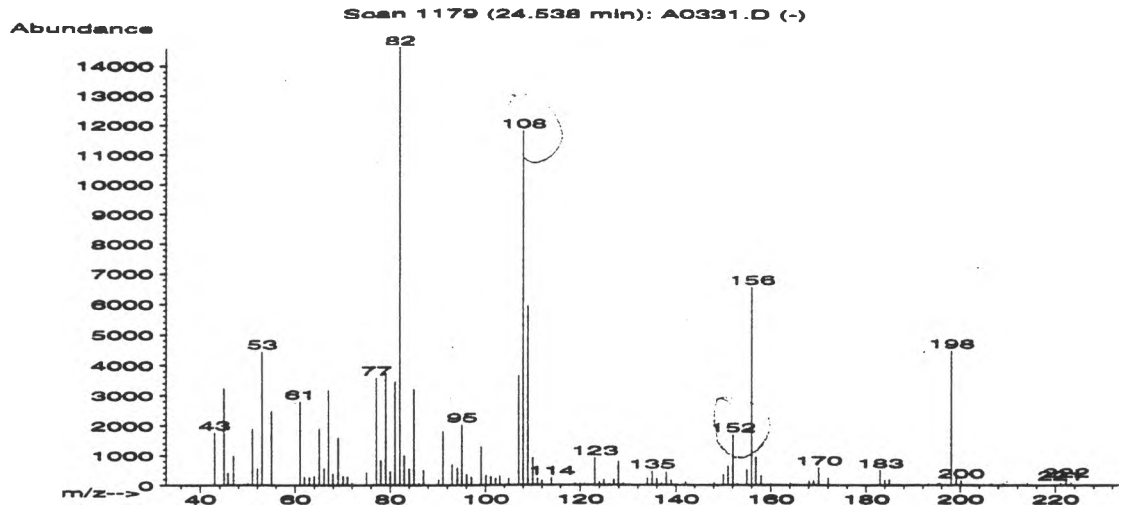
Scan 1125 (23.644 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	N-METHYL-2-PYRIDONE-6-CARBOXYLIC ACID	153	C7H7NO3	27
2.	3,4-Furandicarboxylic acid, 2-methyl-, d	198	C9H10O5	27
3.	2-Chloro-1H-pyrrolizin-1-one	153	C7H4ClNO	25
4.	2-CYANO-4-METHYLPENTENOATE	139	C7H9NO2	22
5.	4-Cyclopentene-1,3-diol, trans-	100	C5H8O2	22
6.	Pentane, 1-(2,2-dichloro-1-methylcyclopr	194	C9H16Cl2	22
7.	Benzene, 1-chloro-4-isocyanato-	153	C7H4ClNO	15
8.	4-Cyclopentene-1,3-diol, cis-	100	C5H8O2	12
9.	Benzene, 1-chloro-2-isocyanato-	153	C7H4ClNO	11
10.	Hydrazine, (4-nitrophenyl)-	153	C6H7N3O2	11
11.	Pyridine, 3-(propylthio)-	153	C8H11NS	11
12.	1,4-Benzenediamine, 2-nitro-	153	C6H7N3O2	10
13.	Benzenamine, 3,5-dimethoxy-	153	C8H11NO2	10
14.	4- AMINOSALICYLIC ACID	153	C7H7NO3	10
15.	Phenol, 4-methyl-2-nitro-	153	C7H7NO3	10
16.	Benzenamine, 3-methyl-N-sulfinyl-	153	C7H7NOS	10
17.	1,3,6-Cycloheptatriene-1-carboxylic acid	198	C8H6O6	9
18.	Benzene, 1-(dichloromethyl)-4-ethyl-	188	C9H10Cl2	9
19.	Benzene, 2-chloro-1-methyl-4-(1-methylet	168	C10H13Cl	9
20.	Phenol, 4-methyl-2-nitro-	153	C7H7NO3	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*27	059864-31-2	13946	33	73	1	99	60	8	0	39	8041
2.	27	006141-60-2	33576	56	98	0	55	60	8	0	39	4197
3.	*25	081400-20-6	13931	34	6	0	92	64	7	10	43	7395
4.	*22	000000-00-0	8868	38	85	0	58	63	5	0	39	2733
5.	*22	000694-47-3	1096	34	78	3	87	63	5	0	39	2733
6.	*22	024551-80-2	31581	35	99	3	157	63	5	0	39	2963
7.	*15	000104-12-1	124067	66	45	2	67	77	2	0	58	7359
8.	*12	029783-26-4	1095	37	69	2	68	63	2	16	37	2733
9.	*11	003320-83-0	13932	60	52	2	67	77	2	0	46	7395
10.	*11	000100-16-3	13924	48	58	3	82	79	2	0	46	7429
11.	*11	026891-62-3	14050	37	54	2	69	79	2	13	43	7310
12.	*10	005307-14-2	13925	45	66	1	70	76	1	0	39	7768
13.	*10	010272-07-8	14032	42	56	2	67	76	1	0	39	6945
14.	*10	000000-00-0	13974	39	73	1	68	70	1	7	36	7446
15.	*10	000119-33-5	124069	46	63	2	94	77	1	13	38	7646
16.	*10	015795-43-4	13940	47	77	3	68	77	1	0	40	7323
17.	9	000099-23-0	33530	47	84	2	70	80	1	0	35	6735
18.	9	054789-29-6	29007	47	76	1	66	77	1	0	37	7401
19.	9	004395-79-3	20286	43	60	1	78	77	1	0	37	7395
20.	* 9	000119-33-5	13954	46	67	3	94	77	1	4	37	7621

Peak 75



Scan 1179 (24.538 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1766	62.00	280	75.05	431	87.00	507
44.95	3228	63.00	262	77.05	3564	90.15	196
45.80	411	64.00	298	78.05	831	91.10	1811
46.95	992	65.00	1889	79.05	3723	93.00	701
49.95	73	66.00	577	80.00	452	94 05	589
50.95	1889	67.00	3167	81.00	3439	95.05	2023
52.00	570	67.95	379	82.00	14579	96.05	363
53.05	4421	69.00	1594	83.00	994	97.00	262
55.05	2484	70.00	299	84.00	552	99.05	1293
57.00	6	70.95	271	85.00	3189	100.05	332
61.00	2782	72.00	76	86.00	73	101.05	291

Scan 1179 (24.538 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
102.05	234	120.00	56	136.00	234	156.00	6554
103.05	307	121.00	55	137.00	83	156.90	950
104.95	219	123.05	924	138.00	428	158.00	319
107.00	3651	124.00	109	139.00	168	160.00	37
108.00	11758	125.00	192	142.05	109	164.15	85
109.00	5936	126.05	48	148.05	102	168.05	151
110.00	926	127.00	198	150.05	348	169.05	153
111.05	219	127.95	802	151.05	644	170.05	589
112.00	152	129.00	67	152.05	1695	172.05	249
114.00	254	134.00	250	153.00	59	173.00	11
118.95	85	135.00	469	155.00	511	183.00	509
184.00	164	209.00	55				
184.90	192	214.05	76				
186.95	27	220.05	30				
193.05	38	221.05	90				
195.20	55	222.20	195				
195.55	77	223.30	88				
198.05	4456						
199.20	525						
200.15	154						
206.20	1						
206.65	61						

Compounds from Proctor and Gamble A0331.D

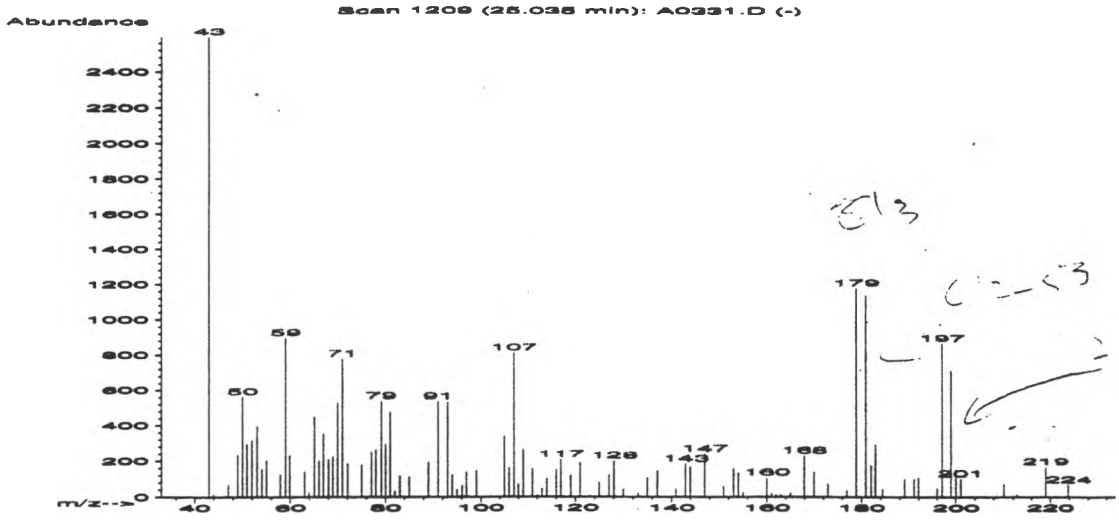
Scan 1179 (24.538 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	**Isopulegone**	152	C10H16O	**46**
2.	Phosphine, (1-methylethyl)phenyl-	152	C9H13P	27
3.	1,2-Benzenediamine	108	C6H8N2	14
4.	2-Pyridinamine, 3-methyl-	108	C6H8N2	14
5.	OROTIC ACID-TRIMETHYL	198	C8H10N2O4	14
6.	1,6-OCTADIENE, 2,5-DIMETHYL-, CIS	138	C10H18	12
7.	2-Cyclohexen-1-one, 4-(3-hydroxy-1-buten	208	C13H20O2	12
8.	4-KETO-.ALPHA.-IONOL	208	C13H20O2	12
9.	1,4-Benzenediamine	108	C6H8N2	10
10.	2-(2-PROPENYL)-FURAN	108	C7H8O	10
11.	2-Pyridinamine, 6-methyl-	108	C6H8N2	10
12.	1H-Pyrrolizine-1-methanol, hexahydro-7-h	157	C8H15NO2	10
13.	Hydrazine, phenyl-	108	C6H8N2	10
14.	Benzene, methoxy-	108	C7H8O	10
15.	Acetic acid, 2-methylphenyl ester	150	C9H10O2	10
16.	2-Pyridinamine, 4-methyl-	108	C6H8N2	10
17.	Phenol, 3-methyl-	108	C7H8O	10
18.	Heptanenitrile	111	C7H13N	10
19.	3-Hexyne	82	C6H10	10
20.	2-Pyridinamine, 4-methyl-	108	C6H8N2	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	029606-79-9	123984	37	58	3	99	41	20	10	43	8714
2.	*27	054722-12-2	13542	33	70	2	59	58	8	11	40	5560
3.	*14	000095-54-5	1904	33	63	1	80	68	2	0	39	5811
4.	*14	001603-40-3	118698	36	60	1	77	68	2	0	39	5840
5.	*14	004116-39-6	128138	33	51	1	99	70	2	1	40	6935
6.	*12	068702-25-0	8725	35	76	3	105	64	2	0	35	7145
7.	12	052210-15-8	38527	44	70	2	72	65	2	7	35	6066
8.	12	034318-21-3	38528	44	85	2	73	65	2	0	35	6058
9.	*10	000106-50-3	118713	32	57	0	65	68	1	0	33	5773
10.	*10	000000-00-0	1912	33	59	0	56	71	1	3	38	5773
11.	*10	001824-81-3	118704	37	45	1	71	73	1	0	39	5746
12.	*10	000520-62-7	124610	40	36	0	77	76	1	0	39	6631
13.	*10	000100-63-0	118706	33	66	2	80	73	1	0	39	5611
14.	*10	000100-66-3	118736	36	46	1	65	73	1	11	40	5593
15.	*10	000533-18-6	12598	41	54	1	57	68	1	16	37	5789
16.	*10	000695-34-1	118700	34	46	0	73	73	1	0	41	5712
17.	*10	000108-39-4	118721	37	69	3	80	74	1	0	39	5365
18.	*10	000629-08-3	118929	34	57	2	90	75	1	13	40	6651
19.	*10	000928-49-4	116762	38	58	2	77	76	1	0	39	6631
20.	* 9	000695-34-1	118701	30	55	1	70	73	1	0	33	5676

Peak 76



Scan 1209 (25.035 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2595	57.95	127	71.00	777	89.00	194
43.90	15	59.00	896	72.05	184	91.05	537
46.95	67	59.90	231	75.00	179	93.00	533
48.95	236	63.00	141	77.05	249	94.00	123
49.95	561	63.90	23	78.00	265	95.00	40
50.95	295	65.10	450	79.05	538	96.05	65
51.95	318	66.05	203	80.00	294	96.95	140
53.05	397	67.00	356	80.95	476	99.05	148
54.05	156	68.05	210	82.00	31	105.00	340
55.00	204	68.95	225	83.00	119	106.00	162
56.95	4	69.95	528	85.00	113	107.00	814

Scan 1209 (25.035 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.00	72	121.95	1	143.95	168	167.95	232
109.00	265	123.05	6	146.95	240	170.05	140
111.00	159	125.00	81	150.95	58	173.00	69
112.00	9	127.05	124	153.00	158	176.95	36
113.00	46	128.05	202	154.00	135	178.90	1180
114.00	105	129.95	42	155.00	25	180.90	1140
115.00	1	133.00	20	160.00	107	182.00	176
116.00	156	135.00	108	161.00	18	182.90	291
116.95	209	137.00	147	161.95	14	184.40	43
119.05	122	140.95	42	163.00	11	189.00	101
121.00	194	142.95	185	165.00	21	191.00	101

Scan 1209 (25.035 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.95	109						
196.00	47						
197.05	869						
198.95	714						
200.05	152						
201.05	102						
210.15	71						
212.90	14						
218.95	167						
223.80	67						

Scan 1209 (25.035 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-PHENYLTHIO-1-ACETOXY-2-PROPANONE	224	C11H12O3S	9
2.	5,9-DIMETHYL-2-(1-METHYLETHYL)-1-CYCLODE	224	C15H28O	9
3.	(3a.alpha.,5a.alpha.,6.alpha.,9aR*)-Hexa	308	C10H13IO3	7
4.	3,4-DIACETYL-2,5-HEXANEDIONE	198	C10H14O4	7
5.	ETHYL-N-P-TOLYCARBAMATE	179	C10H13NO2	7
6.	6-(3'-ACETYL-2'-METHYL-1'-CYCLOPROPEN-1'	222	C14H22O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	9	022198-56-7	45583	44	88	2	86	78	1	0	34	4820
2.	9	004570-15-4	46038	43	74	2	39	77	1	0	34	5298
3.	7	089908-93-0	76213	33	79	1	38	73	1	0	22	5926
4.	7	000000-00-0	33670	33	83	2	67	78	1	0	22	5074
5.	7	000000-00-0	25084	33	87	1	45	73	1	0	21	6104
6.	7	065868-86-2	44823	47	63	3	99	78	1	5	23	4989

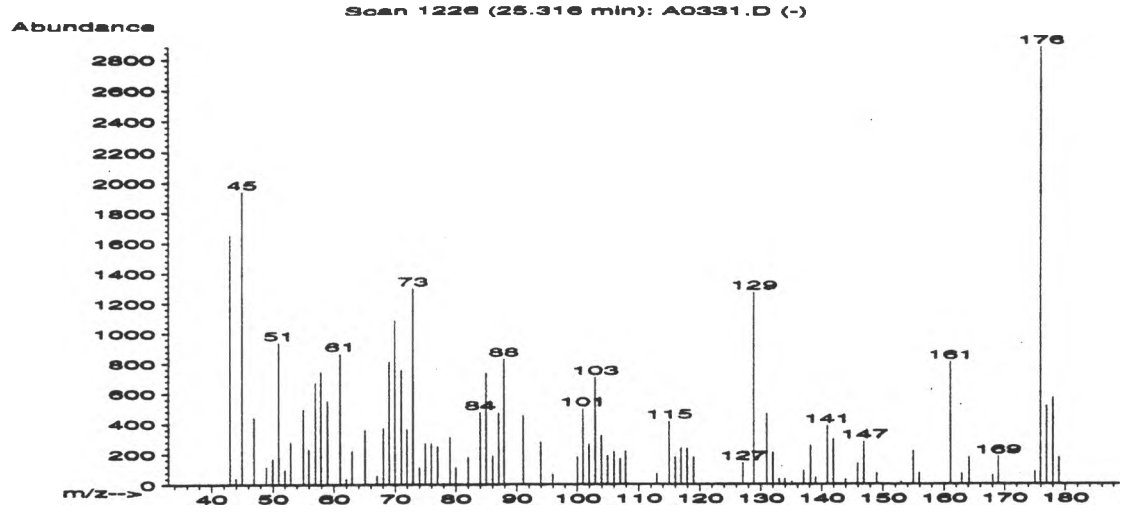
179 + 35
35
214

214
197
17

197
35
232

232
179
53

Peak 77



Scan 1226 (25.316 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1651	57.00	673	71.00	755	84.95	736
43.95	43	57.90	744	71.95	362	86.00	187
44.95	1939	58.95	548	72.95	1297	87.00	473
46.90	440	61.00	866	74.00	114	87.90	830
48.95	117	61.95	37	74.95	273	91.05	455
49.95	168	62.90	220	75.95	272	93.95	281
50.95	937	65.00	357	77.00	251	95.95	67
51.95	99	67.00	58	79.05	312	100.05	181
52.95	280	68.05	369	80.00	113	100.95	499
55.05	496	69.00	814	82.00	178	101.95	267
55.95	231	69.95	1087	84.00	476	102.95	707

Scan 1226 (25.316 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.95	319	127.10	141	141.95	296	164.15	175
104.95	187	128.90	1266	143.95	34	168.05	63
106.00	217	131.00	463	145.95	137	168.95	181
107.00	167	132.00	209	146.95	280	175.05	84
107.90	219	133.00	37	149.00	73	175.95	2881
113.00	72	133.95	40	152.95	19	177.00	511
115.00	415	135.05	19	154.90	216	178.00	563
116.00	179	137.00	90	155.90	78	179.00	173
116.95	237	138.15	255	158.95	1		
117.95	234	139.00	47	161.05	806		
119.00	176	140.95	384	162.95	72		

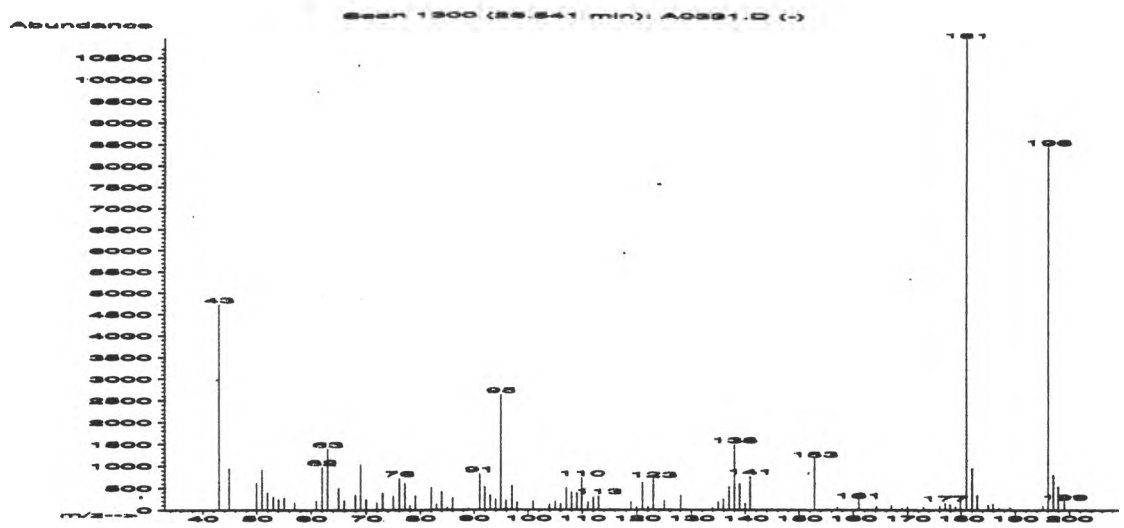
Scan 1226 (25.316 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-METHOXY-1-P-XYLYL-1-PROPENE	176	C12H16O	43
2.	Benzene, 2-(2-methoxy-1-propenyl)-1,4-di	176	C12H16O	43
3.	5-Nitro-3-methylindole	176	C9H8N2O2	27
4.	5-CHLORO-4-HYDROXY-2-(METHYLTHIO)PYRIMID	176	C5H5ClN2OS	25
5.	2-PHENYL-4-METHYL-1,3,4-OXADIAZOL-5-ONE	176	C9H8N2O2	22
6.	4-Isopropenyl-7-methyltricyclo(3.2.1.0)o	176	C12H16O	22
7.	4-HYDRAZINO-1-OXO-1,2-DIHYDROPHTHALAZINE	176	C8H8N4O	22
8.	4-Quinazolinol, 2-methyl-, 3-oxide	176	C9H8N2O2	22
9.	Benzo[b]thiophene, 2,5,7-trimethyl-	176	C11H12S	16
10.	2-PHENYL-5-METHOXY-1,3,4-OXADIAZOLE	176	C9H8N2O2	16
11.	5-Nitro-2-methylindole	176	C9H8N2O2	16
12.	METHYL (Z)-DEC-2-EN-4,6-DIYNOATE	176	C11H12O2	14
13.	1,3,7,11-Cyclotetradecatetraene-5,9,13-t	176	C14H8	12
14.	4H-1-Benzopyran-4-one, 6-hydroxy-2-methy	176	C10H8O3	12
15.	2(3H)-Benzofuranone, 3-(methoxymethylene	176	C10H8O3	12
16.	2H-1-Benzopyran-2-one, 7-methoxy-	176	C10H8O3	10
17.	Phenol, 3-cyclohexyl-	176	C12H16O	10
18.	Quinoxaline, 2-methoxy-, 4-oxide	176	C9H8N2O2	10
19.	4'-METHOXY-2-DIAZOACETOPHENONE	176	C9H8N2O2	10
20.	Ethane, 1,1-diethoxy-	118	C6H14O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	042797-68-2	23947	33	57	2	90	48	18	18	43	7199
2.	*43	053291-93-3	23948	33	60	2	84	50	18	18	43	7199
3.	*27	061861-88-9	23729	37	79	2	81	58	8	0	39	7632
4.	*25	000000-00-0	23559	42	87	3	99	55	7	0	33	7830
5.	*22	000879-60-7	23717	36	73	3	99	64	5	0	39	7051
6.	*22	073036-61-0	24004	35	51	1	99	64	5	11	40	7204
7.	*22	014161-35-4	23659	34	68	1	97	63	5	0	39	7251
8.	*22	054518-07-9	23735	41	66	0	67	63	5	0	39	6925
9.	*16	016587-65-8	23894	41	76	2	81	60	3	7	34	7172
10.	*16	051627-42-0	23721	36	80	3	98	58	3	0	30	7131
11.	*16	007570-47-0	23728	38	89	1	78	58	3	0	33	7616
12.	*14	000505-01-1	23886	46	62	3	99	67	2	14	40	7116
13.	*12	005236-46-4	24083	40	84	3	77	63	2	0	35	7215
14.	*12	022105-12-0	23770	35	77	3	99	63	2	0	35	7032
15.	*12	040800-90-6	23766	28	55	0	72	64	2	2	37	7095
16.	*10	000531-59-9	126469	35	71	3	99	71	1	0	39	6941
17.	*10	001943-95-9	23964	36	46	1	94	70	1	21	37	7110
18.	*10	018916-46-6	23738	38	89	1	67	70	1	0	35	7070
19.	*10	006832-17-3	23710	34	86	2	99	72	1	0	39	6925
20.	10	000105-57-7	119809	47	30	0	56	75	1	2	41	5050

Peak 78



Scan 1300 (26.541 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4728	63.00	1389	77.05	605	92.95	335
44.85	941	65.00	500	78.05	93	93.95	233
49.95	614	66.00	211	79.05	330	94.95	2636
50.95	910	68.05	344	82.00	514	95.90	211
51.95	384	69.00	1034	83.00	138	97.00	559
53.00	288	70.00	234	84.00	413	97.95	177
54.05	236	71.00	6	85.00	54	100.95	192
55.05	276	71.95	172	86.00	276	103.95	135
56.95	166	72.95	383	89.00	36	105.00	192
60.95	203	74.95	313	91.00	820	106.00	141
62.00	976	76.05	720	91.95	538	107.05	508

Scan 1300 (26.541 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.00	402	122.00	78	140.00	150	168.95	40
109.00	384	123.00	704	140.95	771	169.95	71
109.90	729	124.00	9	144.95	34	173.00	61
111.00	174	125.00	204	149.95	15	176.00	84
112.00	281	128.05	329	151.00	21	177.00	163
113.00	317	134.00	49	152.90	1169	177.90	122
115.00	19	135.00	182	157.10	65	178.95	74
116.00	13	135.95	253	159.00	5	179.90	306
118.95	182	137.00	537	161.00	224	181.00	10958
119.95	62	138.00	1492	164.15	79	182.00	960
121.00	624	139.00	605	166.95	101	183.00	332

Scan 1300 (26.541 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
185.00	118						
185.90	138						
187.05	37						
189.00	55						
195.10	94						
196.05	8470						
197.05	807						
197.95	545						
199.05	193						

Compounds from Proctor and Gamble A0331.D

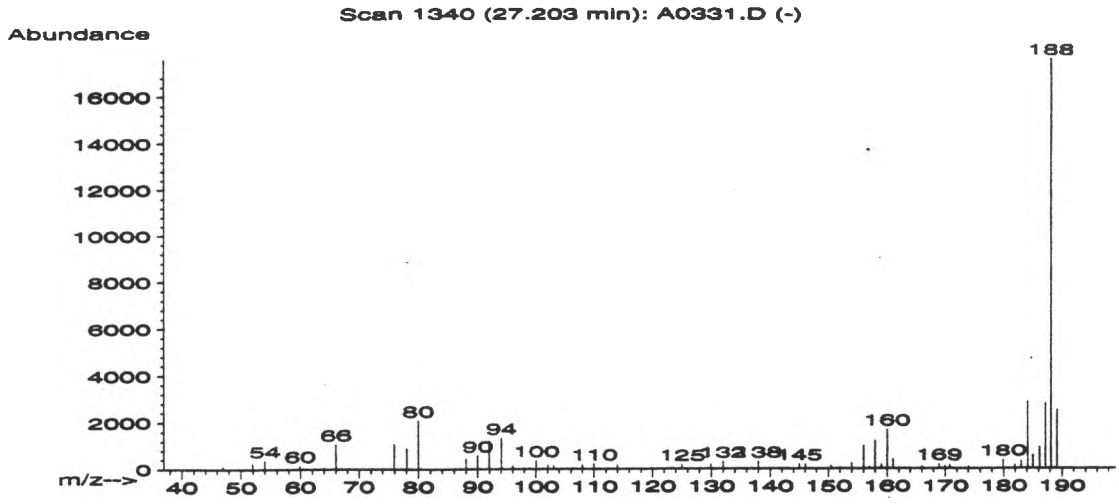
Scan 1300 (26.541 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Silane, (4-methoxyphenoxy)trimethyl-	196	C10H16O2Si	64
2.	Benzaldehyde, 3,4,5-trimethoxy-	196	C10H12O4	50
3.	1-(.alpha.-Hydroxyacetyl)-2-methylcycloh	196	C11H20OSi	45
4.	2-Hydroxy-4,5-dimethoxyacetophenone	196	C10H12O4	45
*5.	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphen	196	C10H12O4	45
6.	Benzaldehyde, 3,4,5-trimethoxy-	196	C10H12O4	45
7.	Benzene, 1,2-dimethyl-4-(phenylmethyl)-	196	C15H16	42
8.	3-Methyl-2-(3-methyl-2-butenyl)furan	196	C11H16OS	38
9.	Benzene, chlorotriethyl-	196	C12H17Cl	36
10.	2-BIPHENYLYL VINYL ETHER	196	C14H12O	32
11.	2-Methyl-2-phenyl-1,3-dithiolane	196	C10H12S2	28
12.	4-AMINOFLUORENE	181	C13H11N	27
13.	Thiazolo[3,2-a]pyridinium, 2,3-dihydro-8	181	C9H11NOS	25
14.	2-Hydroxy-9-fluorenone	196	C13H8O2	22
15.	5-AMINO-ISO-PHTHALIC ACID	181	C8H7NO4	22
16.	6,8-Dimethyl-2(1H)-thioimidazo[1,5-a]-1,	196	C7H8N4OS	17
17.	2-DIMETHYLAMINO-6,7-DIHYDRO-4H,8H-OXAZIN	196	C8H12N4O2	16
18.	Benzoic acid, 3,4-dimethoxy-, methyl est	196	C10H12O4	16
19.	Benzoic acid, 3,5-dimethoxy-, methyl est	196	C10H12O4	16
20.	3,4-DIMETHOXYBENZALDEHYDE OXIME	181	C9H11NO3	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	006689-38-9	32773	50	51	3	99	25	37	0	44	9694
2.	*50	000086-81-7	32715	48	69	2	52	33	25	4	39	9015
3.	*45	000000-00-0	32901	47	36	1	87	25	19	6	33	9671
4.	*45	020628-06-2	32718	41	31	2	67	21	19	2	37	9831
5.	*45	002478-38-8	32719	31	64	2	98	21	19	2	30	9509
6.	*45	000086-81-7	127962	44	94	2	64	25	19	0	35	9320
7.	*42	013540-56-2	128076	36	85	2	84	26	17	0	35	9705
8.	*38	084735-63-7	32811	30	29	1	113	23	14	0	29	9647
9.	*36	031390-10-0	32917	28	87	3	80	26	12	6	29	9610
10.	*32	000000-00-0	33159	35	100	2	77	47	9	0	35	8716
11.	28	005769-02-8	32738	38	92	2	73	39	8	0	29	9590
12.	*27	000000-00-0	26192	34	84	1	67	57	8	0	41	7721
13.	*25	023933-08-6	26008	34	86	3	96	52	7	0	35	7799
14.	*22	006949-73-1	33062	35	74	2	77	62	5	0	39	5941
15.	*22	000000-00-0	25989	43	75	3	99	64	5	0	40	7665
16.	*17	070187-81-4	32568	29	23	2	71	55	3	0	29	6005
17.	*16	074468-22-7	32604	35	78	2	61	57	3	0	35	6001
18.	*16	002150-38-1	127952	40	79	3	56	57	3	0	35	6637
19.	*16	002150-37-0	32691	33	61	1	57	60	3	16	35	5981
20.	*16	002169-98-4	26049	39	75	3	81	59	3	0	33	7715

Peak79



Scan 1340 (27.203 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
46.95	133	88.00	446	108.00	180	150.45	116
51.95	236	90.00	589	110.00	208	152.05	56
54.00	371	91.95	1194	114.00	173	154.00	233
57.90	7	94.05	1330	125.05	182	156.00	984
59.90	148	96.00	121	128.15	24	157.00	89
63.95	58	97.95	48	129.90	194	158.00	1200
66.00	1073	99.00	47	132.00	305	159.05	178
72.95	3	100.05	357	138.00	306	160.00	1670
75.95	1082	102.05	168	142.95	17	161.00	408
78.05	889	103.05	153	145.00	196	162.00	36
80.00	2091	106.00	35	146.05	192	166.00	89

Scan 1340 (27.203 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
168.95	199	188.15	17598				
169.95	100	189.15	2485				
170.80	155						
174.05	85						
179.90	375						
181.95	161						
183.00	323						
184.15	2868						
185.00	561						
186.15	925						
187.15	2780						

Compounds from Proctor and Gamble A0331.D

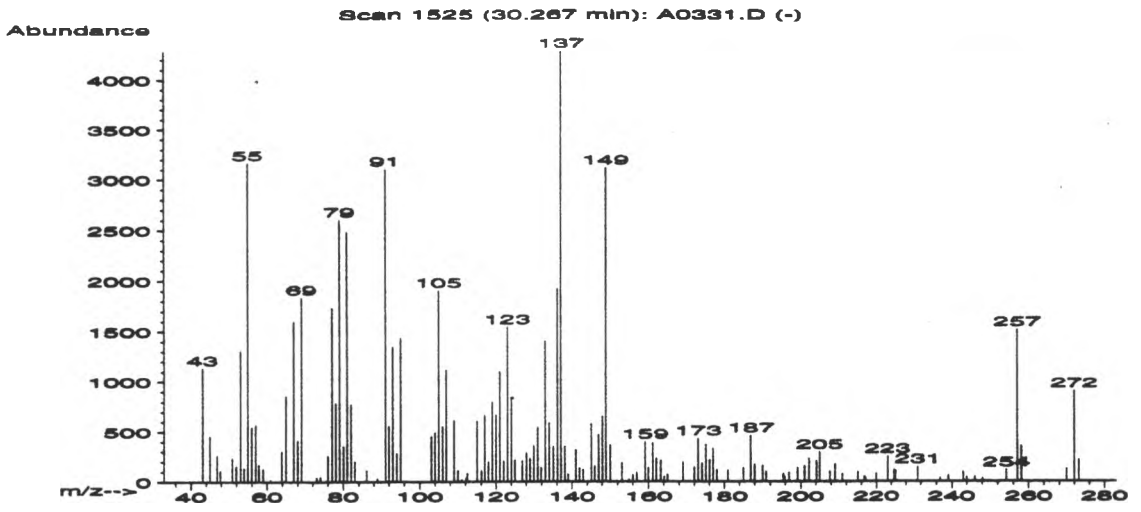
Scan 1340 (27.203 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Anthracene-D10	178	C14D10	87
2.	DECADEUTEROPHENANTHRENE	178	C14D10	78
3.	3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimeth	188	C11H12N2O	53
4.	3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimeth	188	C11H12N2O	53
5.	4-METHYL-2-(3-FLUOROPHENYL)PYRIMIDINE	188	C11H9FN2	53
6.	Phosphonic acid, (3-methyl-3-penten-1-yn	188	C8H13O3P	53
7.	(3-METHYL-3-PENTENE-1-YN)-YL-DIMETHYL-PH	188	C8H13O3P	53
8.	1-PHENYL-4,5-DIMETHYL-4-IMIDAZOLIN-2-ONE	188	C11H12N2O	47
9.	5-Oxazolecarboxamide, 2-phenyl-	188	C10H8N2O2	47
10.	Naphthalene, 2,6-dimethoxy-	188	C12H12O2	47
11.	Benzene, 1-(1-cyclohexen-1-yl)-4-methoxy	188	C13H16O	45
12.	2-Methyl-6-phenyl-2,3,4,5-tetrahydro-3-p	188	C11H12N2O	45
13.	Naphthalene, 1,7-dimethoxy-	188	C12H12O2	40
14.	1,4-Naphthalenedione, 2-methoxy-	188	C11H8O3	40
15.	3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimeth	188	C11H12N2O	40
16.	2,6-Dioxo-1,2,3,5,6,7-hexahydrobenzo[1,2	188	C10H8N2O2	40
17.	Pyrrolo[2,3-b]indole, 1,2,3,3a,8,8a-hexa	188	C12H16N2	38
18.	1-Naphthalenamine, 4-nitro-	188	C10H8N2O2	38
19.	4-HYDROXY-6-PHENYL-3-PYRIDAZONE	188	C10H8N2O2	36
20.	3H-Pyrazol-3-one, 1,2-dihydro-1,5-dimeth	188	C11H12N2O	36

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*87	000000-00-0	24971	82	25	1	95	6	54	8	52	9857
2.	*78	001517-22-2	24973	60	43	1	98	8	46	4	39	9842
3.	*53	000060-80-0	127502	34	79	1	78	30	28	0	41	9705
4.	*53	000060-80-0	29200	36	92	2	99	30	28	0	39	9701
5.	*53	076128-66-0	29193	36	73	1	81	30	28	0	39	9702
6.	*53	022152-34-7	28985	37	57	1	81	30	28	18	40	9740
7.	*53	022152-33-6	28987	37	57	1	82	30	28	18	40	9740
8.	*47	041647-53-4	29205	33	83	3	99	36	20	0	41	9648
9.	*47	039819-42-6	29103	33	83	2	77	40	20	0	41	9581
10.	*47	005486-55-5	29280	35	52	1	71	36	20	1	40	9608
11.	*45	020758-60-5	29353	31	56	2	90	25	19	6	35	9308
12.	*45	003617-20-7	29214	38	51	1	95	23	19	7	36	9675
13.	*40	005309-18-2	29279	35	86	1	94	33	16	0	35	9629
14.	*40	002348-82-5	127495	29	53	1	73	35	16	1	30	8709
15.	*40	000060-80-0	127503	38	41	1	93	33	16	8	37	9696
16.	*40	000000-00-0	29122	37	35	1	70	33	16	0	35	9434
17.	*38	004089-16-1	29325	40	99	1	79	21	14	0	29	8626
18.	*38	000776-34-1	127481	28	40	0	99	36	14	0	33	9593
19.	*36	058884-18-7	29107	31	85	2	79	30	12	0	29	9682
20.	*36	000060-80-0	127499	31	93	1	99	28	12	0	29	9735

Peak 80



Scan 1525 (30.267 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1136	57.90	169	77.05	1729	93.00	1345
44.95	455	59.00	125	78.05	781	94.05	282
46.95	262	60.90	20	79.05	2599	95.00	1435
47.80	109	63.90	303	80.05	352	103.05	451
50.95	233	65.00	853	81.00	2479	104.00	490
51.95	155	67.00	1596	82.00	768	105.00	1904
53.05	1310	68.00	411	83.00	199	106.00	551
54.00	135	69.00	1833	86.15	112	107.00	1121
55.00	3166	73.00	40	88.95	30	109.00	613
56.00	544	74.00	47	91.05	3100	110.00	114
57.00	567	75.95	256	91.95	553	111.05	20

Scan 1525 (30.267 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
112.10	39	124.05	845	136.15	1922	148.95	3113
112.50	85	125.05	215	137.15	4285	150.05	368
115.00	604	127.00	211	138.10	358	152.00	4
116.10	111	128.05	292	139.00	76	153.15	189
117.00	665	128.95	230	141.05	315	154.95	25
117.95	197	130.00	360	141.95	135	156.00	70
119.00	794	131.00	540	142.95	120	157.00	90
120.05	668	131.90	141	145.05	578	159.15	400
121.05	1101	133.00	1405	146.05	159	160.00	141
122.05	207	134.00	588	147.05	467	161.10	386
123.05	1543	135.05	351	148.05	657	162.00	233

Scan 1525 (30.267 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.15	212	180.90	113	202.15	228	223.05	253
164.05	47	185.05	141	204.15	207	224.80	116
164.95	71	187.00	462	205.00	296	225.20	108
169.05	193	188.00	171	207.65	102	231.15	150
172.05	143	190.05	158	207.95	9	236.95	34
173.05	430	190.95	102	209.00	176	239.05	61
174.05	186	195.45	78	211.00	77	243.05	96
175.05	367	195.80	50	215.05	93	243.95	46
176.05	215	196.95	90	216.70	51	246.05	49
177.00	331	199.20	141	217.10	29	248.05	34
178.00	113	200.95	155	219.95	79	254.25	118

Scan 1525 (30.267 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
256.20	9						

257.15	1519
258.15	354
269.95	128
272.05	908
273.20	216

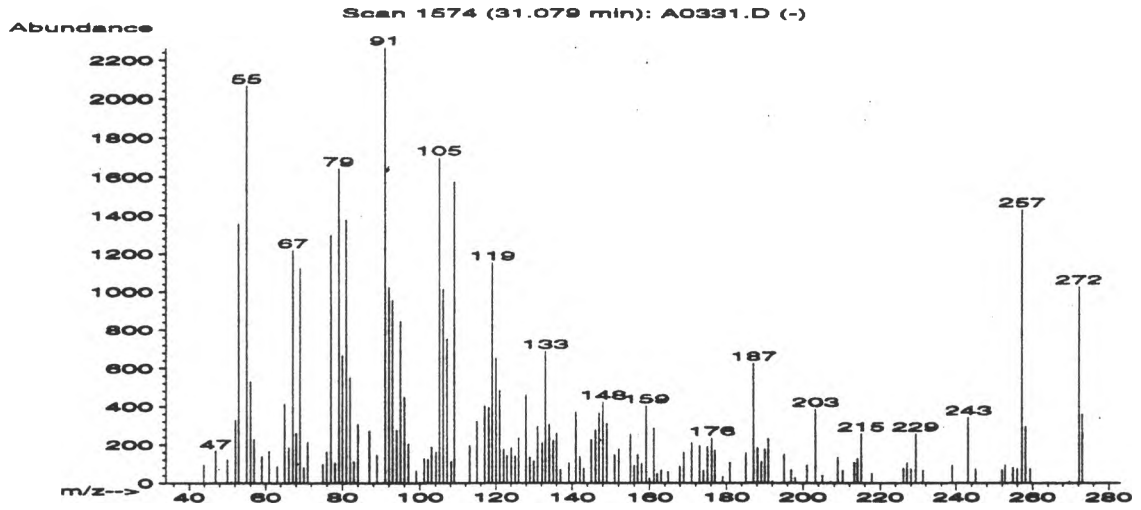
Scan 1525 (30.267 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Sandaracopimaradiene	272	C20H32	89
2.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	38
3.	Androst-5-en-4-one	272	C19H28O	35
4.	Androst-16-en-3-one, (5.alpha.)-	272	C19H28O	30
5.	Phenol, 4-amino-2,5-dimethyl-	137	C8H11NO	27
6.	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	25
7.	5.BETA.-ANDROST-16-ENE-3-ONE	272	C19H28O	20
8.	4a(2H)-Naphthalenecarboxylic acid, octah	196	C12H20O2	16
9.	2-AMINO-4,5,6,7-D4-BENZIMIDAOLE	133	C7H3D4N3	16
10.	Albicanol	222	C15H26O	16
11.	Benzene, 1-methyl-4-nitro-	137	C7H7NO2	14
12.	Benzene, 1-methyl-4-nitro-	137	C7H7NO2	14
13.	Tricyclo[7.1.1.0(4,9)]undecan-10-one or	164	C11H16O	14
14.	1-Buten-1-ol, 2-methyl-4-(2,6,6-trimethy	236	C15H24O2	12
15.	Androstan-3-one, 17-(acetyloxy)-, (5.alp	332	C21H32O3	12
16.	HYDROCINNAMALDEHYDE-.ALPHA.-D2	134	C9H8D2O	11
17.	Pyridinium, 1-(acetylamino)-2,6-dimethyl	164	C9H12N2O	10
18.	trans-syn-cis-Tricyclo[7.3.0.0(2,6)]dode	178	C12H18O	10
19.	2-METHYL-3-.BETA.-FURYL PROPENAL	136	C8H8O2	10
20.	2-Methyl-1-(isopropylamino)-1-cyanobuten	152	C9H16N2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*89	001686-56-2	132292	124	46	1	87	23	56	0	91	8611
2.	38	007683-64-9	136174	75	98	3	86	40	14	16	37	7684
3.	*35	013583-72-7	132273	87	103	2	51	53	11	18	42	8099
4.	*30	018339-16-7	64403	75	89	1	32	61	9	21	60	5453
5.	*27	003096-71-7	8316	33	72	2	90	59	8	0	39	7183
6.	*25	020070-61-5	132290	66	97	0	35	73	7	0	64	6589
7.	*20	018339-16-7	64404	67	97	1	32	66	4	0	58	6569
8.	16	062338-25-4	33008	43	90	3	99	58	3	0	35	7305
9.	*16	000000-00-0	7100	42	48	2	85	58	3	8	37	7240
10.	16	054632-04-1	45030	43	62	2	89	60	3	0	37	7238
11.	*14	000099-99-0	122130	35	61	0	72	70	2	0	39	6724
12.	*14	000099-99-0	122129	35	75	2	131	66	2	0	39	6733
13.	*14	000000-00-0	18693	53	32	0	45	70	2	5	38	4564
14.	12	021730-91-6	50874	44	79	1	72	61	2	0	37	7142
15.	12	001164-91-6	83552	73	105	1	42	63	2	0	35	5806
16.	*11	029372-33-6	7370	48	59	3	125	78	2	0	44	3596
17.	10	031020-35-6	18363	46	56	2	58	78	1	9	38	5145
18.	10	073306-78-2	24912	43	80	2	70	66	1	0	37	7293
19.	*10	028043-36-9	7787	35	71	2	55	78	1	0	39	3892
20.	10	066102-53-2	13548	44	62	2	66	66	1	0	37	6801

Peak 81



Scan 1574 (31.079 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.85	98	63.00	88	78.05	106	93.00	956
46.95	167	65.00	412	79.05	1638	94.00	275
49.95	122	66.05	185	80.00	665	95.00	845
50.95	6	67.15	1218	81.00	1377	96.00	449
52.05	329	68.00	258	82.00	551	97.00	206
52.95	1358	69.00	1124	83.00	112	99.00	66
55.05	2065	70.00	83	84.00	306	101.05	128
56.00	530	71.05	213	87.00	272	102.05	122
57.00	229	74.95	97	88.95	146	103.00	190
58.95	140	75.95	162	91.05	2262	104.05	159
60.95	166	77.05	1297	92.05	1021	105.00	1691

Scan 1574 (31.079 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
106.00	1014	122.05	176	134.05	305	148.05	422
107.00	753	123.00	144	135.00	223	149.00	311
108.10	114	124.05	184	136.00	258	151.00	147
109.00	1570	125.05	141	137.00	71	152.05	177
113.00	196	126.05	237	139.15	107	155.00	255
115.00	324	127.95	460	140.95	371	156.00	94
117.00	402	128.95	134	142.00	137	156.95	148
118.05	394	130.00	115	143.05	77	158.00	102
119.05	1152	131.00	295	144.95	226	159.15	402
120.05	652	132.15	208	146.05	277	159.95	26
121.00	484	133.00	689	147.00	365	161.15	285

Scan 1574 (31.079 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
162.00	49	178.95	32	197.95	29	226.00	77
163.00	67	180.90	108	201.05	94	226.90	107
164.90	58	185.15	155	203.25	386	228.00	73
167.95	87	187.15	625	205.00	38	229.25	257
168.95	159	188.15	184	207.10	7	230.95	5
170.95	210	189.15	112	209.00	135	231.25	65
173.05	196	190.05	177	210.25	67	238.95	94
174.05	66	191.05	233	213.15	107	243.15	343
175.05	190	192.05	8	214.05	127	245.05	73
176.20	234	195.05	149	215.05	256	251.90	69
177.05	171	196.95	69	217.70	50	252.75	95

Scan 1574 (31.079 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
254.75	81						

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   255.90        75
   257.15      1432
   258.15       296
   259.40        74
   269.70        12
   272.20      1030
   273.05       360
Scan 1574 (31.079 min): A0331.D


PBM Search of library D:\DATABASE\WILEY138.L

    Name                                          MolWt Formula            Qual
 1. (E)-4-Ethyl-1,3-dimethyl-5-(3,4-dimethyl      272 C16H20N2O2            72
 2. (Z)-4-Ethyl-1,3-dimethyl-5-(3,4-dimethyl      272 C16H20N2O2            64
 3. (3.alpha.,6a.alpha.,6b.beta.,10.beta.,12      272 C18H24O2              55
 4. Kaur-16-ene, (8.beta.,13.beta.)-              272 C20H32                53
 5. (Z)-3-(9-BORABICYCLO[3.3.1]NON-9-YL)-4-D      272 C18H34B2              38
 6. Isopimaradiene                                272 C20H32                38
 7. 1(3H)-Isobenzofuranone, 3a,4,5,7a-tetrah      182 C10H14O3              27
 8. trans-Caryophyllene                           204 C15H24                27
 9. 5,5'-OXY-DIMETHYLENE-BIS(2-FURALDEHYDE)       234 C12H10O5              25
10. Androst-16-en-3-one, (5.alpha.)-              272 C19H28O               25
11. N-(4-METHOXYBENZENESULFONYL)AZETIDIN-3-O      241 C10H11NO4S            25
12. Phenol, 3-amino-                              109 C6H7NO                25
13. 4,4-Dimethyltricyclo(3,2,1.0)octan-6-one      150 C10H14O               22
14. Dimethyltriphenylmethane                      272 C21H20                22
15. Trachylobane                                  272 C20H32                18
16. Anodendrine, iodide, methyl ester             365 C14H24INO2            12
17. (-)-4-oxo-14-norvitrane                       206 C14H22O               12
18. 3.BETA.-HYDROXY-ANDROST-5,16-ENE              272 C19H28O               11
19. Androst-5-en-4-one                            272 C19H28O               11
20. Androst-8-en-11-one, (5.alpha.)-              272 C19H28O               10

    Prob    CAS#        Ref#   K  dK Flag   %  Con C_1 Tilt R_IV  XCORR
 1.*72 087233-18-9     64272  44  40    0  56   16  42    0   44   5369
 2.*64 087233-16-7     64271  37  46    0  56   16  37    0   41   5370
 3.*55 071370-29-1     64348  85  95    2 106   43  29    0   80   6641
 4.*53 020070-61-5    132290  97  93    2  61   75  28    0   93   7054
 5.*38 000000-00-0     64371  44 119    3 211   47  14    0   39   5742
 6.*38 001686-66-4    132293  96  98    2  66   47  14    8   42   8702
 7. 27 054346-06-4     26554  58  65    3 384   59   8    0   39   5267
 8. 27 000087-44-5    128687  54  98    0  68   56   8    0   39   6037
 9. 25 007389-38-0     49777  45  74    0  62   54   7    6   34   5925
10.*25 018339-16-7     64403  83  92    1  51   77   7   30   72   5363
11. 25 082380-60-7     52849  47 102    3 118   54   7    0   34   5012
12.*25 000591-27-5      2058  45  65    2  61   54   7   10   35   5095
13. 22 068276-48-2     12871  54  57    0  68   63   5    0   39   4017
14.*22 000000-00-0     64480  45  80    1  49   64   5    0   40   5381
15.*18 005282-35-9     64471  65 131    2  54   68   3    0   50   6929
16. 12 027510-47-0     91336  45 126    2  53   63   2    0   35   4254
17. 12 077284-02-7     37648  44  77    2  55   63   2    0   37   4017
18.*11 000000-00-0    132279  72 119    3  75   78   2    0   44   6737
19.*11 013583-72-7    132273  56 118    2  49   72   2    0   49   7664
20.*10 054498-82-7     64401  43 134    3  77   75   1    0   39   6241
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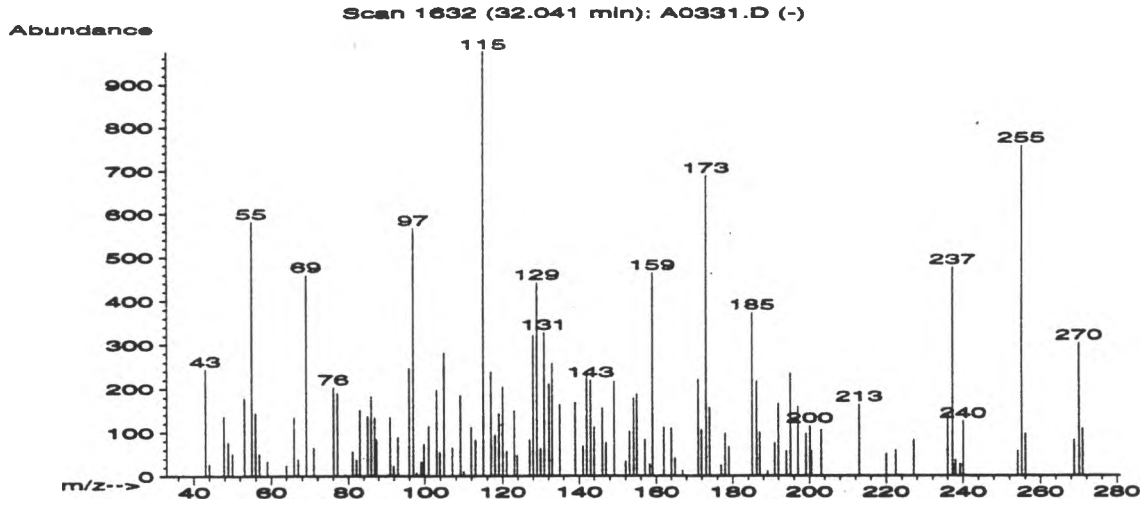
Peak 82



Scan 1632 (32.041 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	244	65.90	134	86.00	183	100.95	115
43.95	28	67.00	38	86.90	134	103.00	197
47.80	136	69.05	459	87.40	83	103.80	55
48.90	77	71.00	65	91.00	134	104.95	282
49.95	51	76.05	203	91.95	23	107.00	65
53.05	178	77.05	190	93.00	90	109.10	184
55.00	582	79.05	4	95.95	247	110.00	10
55.95	144	81.00	56	97.05	566	111.90	112
56.95	51	82.00	37	97.90	7	113.00	83
59.00	34	82.95	151	99.05	32	115.00	975
63.95	24	85.00	137	99.70	73	117.00	238

Scan 1632 (32.041 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.05	94	132.15	212	152.00	34	171.05	221
119.05	143	132.95	258	153.00	102	171.95	106
120.05	204	135.00	164	154.15	178	173.05	688
121.05	56	139.05	168	155.00	187	174.05	157
123.05	150	141.05	69	157.00	84	176.95	25
123.80	48	142.05	238	158.20	27	177.95	98
127.05	83	143.00	220	159.00	464	179.00	67
128.00	322	143.95	112	162.00	112	185.00	373
129.00	442	146.05	157	164.00	110	186.15	218
129.95	63	146.95	76	164.95	41	187.00	100
130.90	328	149.05	218	166.95	13	189.10	11

Scan 1632 (32.041 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.00	75	222.45	59	270.05	304		
191.95	166	227.15	83	270.95	108		
193.95	57	236.00	144				
195.05	235	237.25	477				
197.05	159	237.95	36				
199.15	97	239.25	28				
200.20	115	240.05	126				
200.55	57	254.10	58				
203.15	106	255.15	759				
213.00	164	256.10	96				
220.05	52	268.80	82				

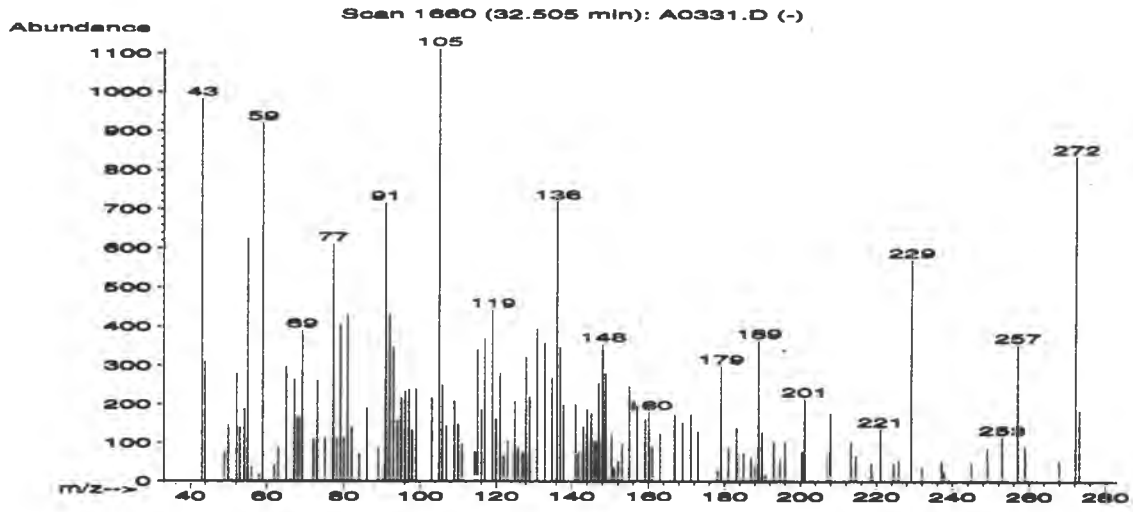
Scan 1632 (32.041 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenanthrene, 1,2,3,4,4a,9,10,10a-octahy	270	C20H30	38
2.	Phenanthrene, 1,2,3,4,4a,9,10,10a-octahy	270	C20H30	14
3.	2,2-Dibromo-1-phenylcyclopropanecarboxyl	240	C10H9BrO2	11
4.	.ALPHA.-D-GLUCOFURANOSE CYCLIC(1,2-METHA	313	C13H23B2O7	10
5.	3,4,5-TRIMETHYL-1-PHENYL-4,5,6,7-TETRAHY	270	C15H18N4O	9
6.	Phenanthrene, 1,2,3,4,4a,9,10,10a-octahy	270	C20H30	9
7.	8-Methyl-2-oxo-2H-pyrano[2,3-b]quinoline	255	C14H9NO4	9
8.	1,3-Dioxane, 4,5-dimethyl-2-pentadecyl-	326	C21H42O2	9
9.	Decanamide, N,N-diethyl-	227	C14H29NO	9
10.	3-METHOXY-4'-NITROSTILBENE	255	C15H13NO3	8
11.	2-Pentenedioic acid, 2-methoxy-, dimethy	188	C8H12O5	8
12.	Silane, trioctyl-	368	C24H52Si	7
13.	3-METHOXY-5'-NITROSTILBENE	255	C15H13NO3	7
14.	Boric acid (H3BO3), tris(1-methylethyl)	188	C9H21BO3	7
15.	DIMETHYL ESTER OF 3-OXO-ADIPIC ACID	188	C8H12O5	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	019407-28-4	132234	33	30	1	77	46	14	0	39	6104
2.	*14	019407-28-4	63774	35	102	1	77	69	2	0	39	6066
3.	*11	093590-95-5	52309	37	71	0	93	80	2	2	43	5481
4.	10	000000-00-0	77889	58	98	2	71	70	1	15	37	5694
5.	9	064899-18-9	63493	47	115	1	62	80	1	0	34	4389
6.	* 9	019407-28-4	132235	42	123	3	107	73	1	0	33	6925
7.	* 9	080231-70-5	58484	32	35	0	60	73	1	0	33	4267
8.	9	056599-32-7	81841	46	93	1	99	79	1	0	37	5781
9.	* 9	002602-61-1	47217	35	93	1	87	80	1	0	35	5598
10.	* 8	000000-00-0	58518	28	83	2	56	69	1	0	29	4267
11.	8	056009-33-7	127451	51	84	1	68	69	1	0	27	6354
12.	7	018765-09-8	92090	42	131	3	68	76	1	0	29	4993
13.	* 7	000000-00-0	58517	30	115	2	56	80	1	0	29	4267
14.	7	005419-55-6	29085	36	99	3	70	79	1	0	20	5217
15.	7	000000-00-0	28971	36	94	2	74	76	1	0	21	6278

Peak 83



Scan 1660 (32.505 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	983	59.00	921	77.05	610	92.05	433
43.90	310	61.95	41	78.00	111	93.00	348
48.85	79	62.90	88	79.05	405	94.05	158
50.00	147	65.00	297	79.95	114	95.00	217
50.95	5	66.10	9	81.00	431	96.05	234
52.20	280	67.00	265	82.05	140	97.05	239
53.00	142	68.05	167	84.00	71	97.95	133
54.20	188	69.00	390	86.00	191	98.95	240
55.05	625	71.95	110	89.00	86	103.05	218
56.00	39	72.95	261	90.25	43	105.00	1112
58.00	18	75.00	113	91.00	715	105.90	250

Scan 1660 (32.505 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	145	122.05	67	137.00	348	150.30	123
109.00	209	123.05	106	138.00	199	151.00	34
110.05	149	125.05	209	141.00	201	152.00	52
111.00	95	125.95	89	141.80	77	153.00	98
114.25	77	127.00	75	143.05	144	155.00	246
115.00	342	128.00	322	143.95	187	156.00	3
116.05	186	129.00	221	145.05	178	157.00	194
117.00	370	130.95	395	146.05	104	159.10	161
119.00	442	133.00	360	147.00	254	160.15	180
119.95	163	134.95	269	148.05	355	161.00	91
121.05	281	136.15	719	148.80	281	163.05	123

Scan 1660 (32.505 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
166.95	173	189.00	365	214.55	65	244.95	48
168.95	153	189.95	128	218.55	49	249.05	88
171.05	175	191.00	16	218.95	16	253.00	116
173.00	130	193.05	102	221.05	137	257.00	355
178.00	28	194.70	59	224.45	48	259.00	92
179.00	299	195.95	103	225.75	56	267.95	53
181.00	88	200.45	78	229.15	572	272.20	837
183.15	140	201.20	215	232.00	37	273.20	185
185.05	74	207.05	76	237.15	52		
187.00	64	207.95	178	237.80	26		
188.10	41	213.25	103	239.15	7		

Scan 1660 (32.505 min): A0331.D

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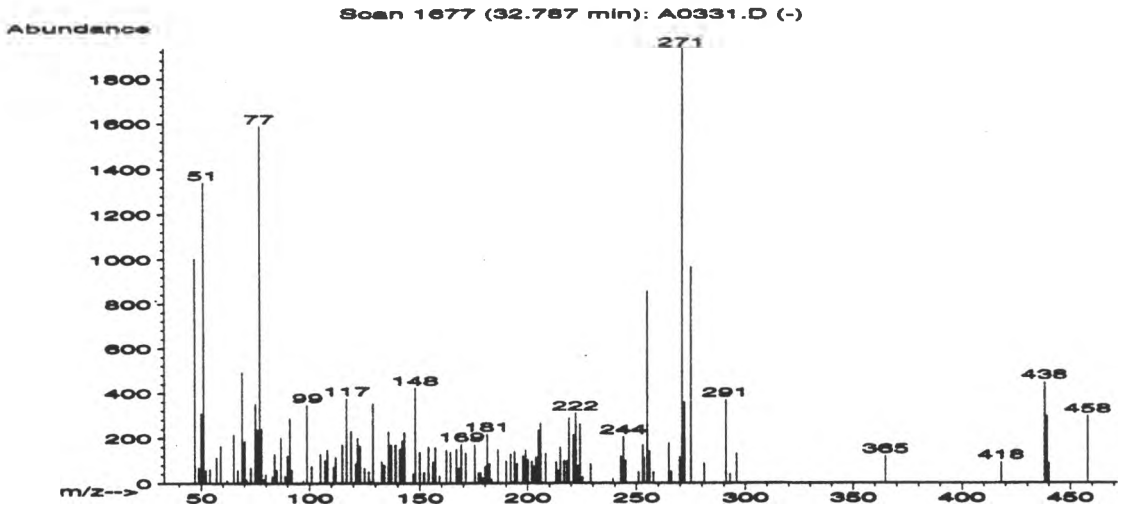
	Name	MolWt	Formula	Qual
1.	3,4,3',3'-BIS(TETRAMETHYLENE)BIFURANDION	272	C16H16O4	38
2.	6-METHYL-4,5-DIPHENYL-4H-CYCLOPENTA[B]FU	272	C20H16O	27
3.	Benzoic acid, 2-hydroxy-6-methyl-4-(phen	272	C16H16O4	27
4.	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	25
5.	ANTI,SYN,ANTI-3,3,6,6,9,9,12,12-OCTAMETH	272	C20H32	22
6.	Benz[3,4]anthra[1,2-b]oxirene, 1a,11b-di	272	C20H16O	22
7.	4-HYDROXY-3-(3-METHOXY BENZOYL)BENZOIC A	272	C15H12O5	22
8.	Benzene, ethenyl-, dimer	208	C16H16	20
9.	Cembrene-C	272	C20H32	14
10.	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	14
11.	1,2,3,4-Phenazinetetrol, 7,8-dimethyl-	272	C14H12N2O4	14
12.	CIS-8,9-DIPHENYL-ENDO-TRICYCLO(6.1.0.0*2	272	C21H20	14
13.	Benzoic acid, 4-methyl-	136	C8H8O2	11
14.	s-Triazolo[4,3-a]pyrazine, 5,6-diphenyl-	272	C17H12N4	11
15.	Estra-1,3,5(10)-triene-3,17-diol (17.bet	272	C18H24O2	11
16.	Androst-16-en-3-one, (5.alpha.)-	272	C19H28O	11
17.	Benzoic acid, 4-methyl-	136	C8H8O2	10
18.	3.BETA.-HYDROXY-ANDROST-5,16-ENE	272	C19H28O	10
19.	Perylene, eicosahydro-	272	C20H32	10
20.	Estra-1,3,5(10)-triene-3,17-diol (17.bet	272	C18H24O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	030839-75-9	64242	71	94	1	71	60	14	0	53	5386
2.	*27	086738-92-3	64430	36	110	1	73	57	8	0	39	5756
3.	*27	022375-05-9	64238	40	71	0	64	60	8	0	39	5434
4.	*25	020070-61-5	64458	66	123	2	60	61	7	0	44	6902
5.	*22	000000-00-0	64473	65	127	3	63	65	5	0	39	6595
6.	*22	039834-38-3	64412	45	129	2	73	63	5	0	39	6650
7.	*22	068595-45-9	64181	35	105	0	75	62	5	0	41	5271
8.	*20	025247-68-1	38803	82	81	2	58	70	4	41	58	3012
9.	*14	064363-64-0	64437	47	117	3	135	68	2	0	40	6147
10.	*14	020070-61-5	132290	75	112	2	52	70	2	16	42	6027
11.	*14	023774-09-6	64141	33	116	0	75	66	2	0	41	5217
12.	*14	000000-00-0	64491	62	77	0	62	67	2	15	40	4910
13.	*11	000099-94-5	121826	48	47	0	61	79	2	0	46	5120
14.	*11	006969-76-2	64293	49	102	1	71	78	2	0	44	5093
15.	*11	000050-28-2	132266	57	93	1	57	79	2	0	49	4910
16.	*11	018339-16-7	132275	69	102	1	62	79	2	0	44	5121
17.	*10	000099-94-5	7791	38	58	0	52	80	1	0	39	5216
18.	*10	000000-00-0	64406	63	129	3	65	79	1	0	39	5223
19.	*10	047041-72-5	132296	48	112	1	72	75	1	0	39	6147
20.	*10	000050-28-2	64362	48	120	1	50	79	1	0	39	4911

Peak 84



Scan 1677 (32.787 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
46.95	1001	67.05	58	83.00	31	105.00	130
48.80	69	68.95	491	84.00	128	107.05	102
49.95	309	70.05	186	85.00	60	108.00	149
50.95	1340	70.95	16	86.90	200	111.00	73
52.00	56	72.95	69	89.00	32	111.90	115
53.95	62	75.00	350	90.00	121	115.00	171
57.00	114	75.95	238	91.00	287	115.95	2
59.00	164	77.05	1588	91.95	59	116.95	377
61.95	13	78.00	241	97.05	11	119.05	231
62.95	1	79.05	18	98.95	348	121.05	87
65.00	215	79.90	39	100.95	77	121.95	199

Scan 1677 (32.787 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.00	165	142.05	189	164.00	139	182.15	87
125.05	68	143.00	225	166.85	151	183.05	19
127.00	52	147.00	42	167.95	69	186.00	149
128.00	8	147.95	424	169.05	174	189.95	100
128.95	353	150.05	139	171.05	135	192.05	130
133.00	97	151.95	48	175.20	170	193.00	5
134.05	79	153.90	162	177.00	45	193.95	142
136.00	228	156.00	94	177.90	47	195.05	87
137.10	169	157.00	159	178.95	25	197.95	122
139.00	171	158.95	33	180.00	75	199.05	147
140.95	152	162.00	147	181.00	218	200.20	105

Scan 1677 (32.787 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
202.00	98	219.05	287	251.00	49	274.90	962
203.00	75	221.05	213	252.90	170	281.00	88
203.90	116	222.05	311	253.50	112	290.85	371
205.00	233	223.10	76	255.00	854	292.80	40
206.00	267	224.05	263	256.00	141	295.80	133
208.15	133	225.15	29	257.90	49	364.80	121
213.00	95	229.00	86	264.95	177	417.95	94
213.80	57	239.15	20	265.95	52	437.95	449
214.95	159	242.80	118	269.80	115	439.05	295
216.80	101	244.05	207	270.95	1933	439.95	90
218.05	99	245.05	102	271.95	359	457.95	297

Scan 1677 (32.787 min): A0331.D

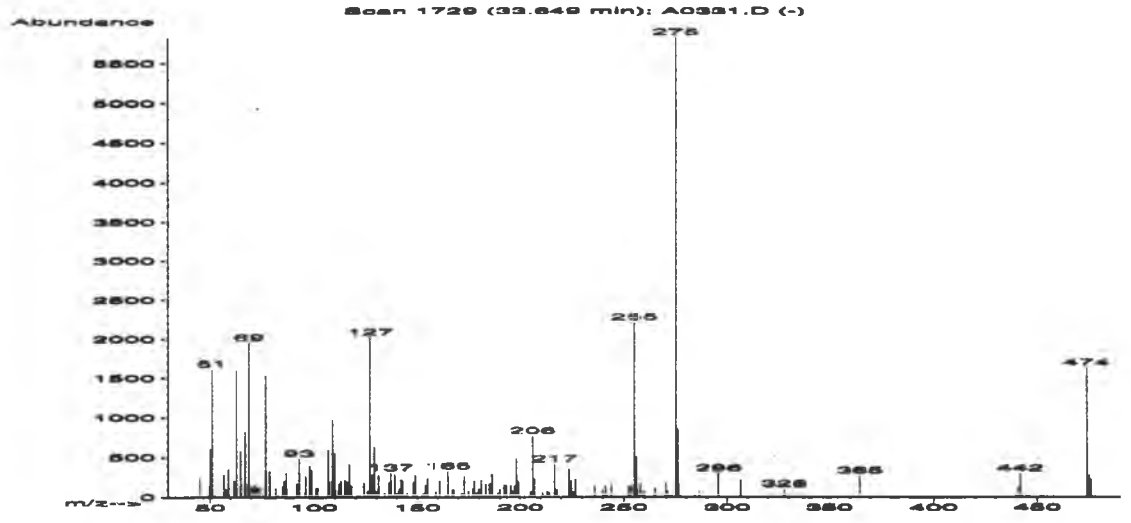
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzenamine, N-[(pentafluorophenyl)methy	271	C13H6F5N	35
2.	Isoxazole, 4-iodo-3-phenyl-	271	C9H6INO	25
3.	Pregn-14-en-3-one, (5.beta.)-	300	C21H32O	10
4.	3-Methoxy-N-methylmorphinan	271	C18H25NO	10
5.	Oxazole, 2-(1-naphthalenyl)-5-phenyl-	271	C19H13NO	10
6.	Crinan-3-ol, 1,2-didehydro-, (3.alpha.)-	271	C16H17NO3	10
7.	4-EPIDEHYDROABIETOL	286	C20H30O	9
8.	Podocarpa-8,11,13-trien-17-oic acid, 12-	344	C22H32O3	9
9.	Ethyl ester of 2,2-Dimethyl-5-(N-methyla	272	C16H20N2O2	9
10.	Silane, dimethyl-2-propenyl(tetradecylox	312	C19H40OSi	9
11.	7-AMINO-2-ETHYL-1-PROPYL-5-(TRIFLUOROMET	271	C13H16F3N3	9
12.	Trichostachine	271	C16H17NO3	9
13.	Crinan-3-ol, 1,2-didehydro-, (3.alpha.)-	271	C16H17NO3	9
14.	DEOXODEOXYDIHYDROMETATHEBAINONE	271	C18H25NO	9
15.	Pregn-15-en-20-one, 17-methyl-, (5.alpha	314	C22H34O	7
16.	13-ISOPROPYLPODOCARPEN-12-OL-20-AL	300	C20H28O2	7
17.	Chol-4-en-24-oic acid, 12-hydroxy-3-oxo-	402	C25H38O4	7
18.	Totarol	286	C20H30O	7
19.	Totarol	286	C20H30O	7
20.	TRIS-(2.4.6-TRIDEUTEROPHENYL)PHOSPHINE	262	C18H6D9P	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	002341-86-8	63843	44	94	2	89	53	11	0	40	8129
2.	*25	023253-50-1	63806	39	103	1	97	53	7	4	34	7993
3.	10	054411-79-9	74059	55	101	1	67	76	1	18	38	6292
4.	*10	000125-70-2	63946	37	141	3	80	73	1	0	39	6292
5.	*10	000846-63-9	63964	40	102	3	92	70	1	0	35	7135
6.	*10	000510-67-8	63893	44	123	3	91	76	1	0	40	6292
7.	9	024035-43-6	132899	47	127	2	84	75	1	0	37	6537
8.	9	024067-43-4	86621	47	105	2	99	76	1	0	34	6292
9.	* 9	085937-68-4	64265	42	99	2	71	75	1	0	33	6863
10.	9	077774-33-5	77726	46	84	3	77	73	1	0	37	6292
11.	* 9	069145-21-7	63846	29	77	1	95	76	1	3	30	6292
12.	* 9	025924-78-1	63891	34	74	1	94	76	1	9	32	6292
13.	* 9	000510-67-8	132241	38	128	3	87	76	1	0	35	6292
14.	* 9	000000-00-0	63951	40	136	3	71	76	1	0	35	6292
15.	7	054411-97-1	78485	38	122	3	96	76	1	0	29	6292
16.	7	000000-00-0	74009	55	93	1	71	76	1	0	27	6292
17.	7	019684-72-1	136059	33	126	0	70	76	1	0	25	6292
18.	7	000511-15-9	132898	42	112	2	73	76	1	0	28	6292
19.	7	000511-15-9	69373	36	120	2	69	76	1	0	21	6292
20.	* 7	002937-10-2	60602	31	122	1	73	76	1	0	29	6292

Peak 65

Compounds from Proctor and Gamble A0331.D



Scan 1729 (33.649 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	18	65.00	578	79.05	329	98.95	342
44.90	237	67.15	824	82.00	116	100.95	112
48.95	143	67.95	158	83.00	21	101.95	120
49.95	599	69.00	1953	85.05	141	106.95	592
50.95	1615	70.05	77	85.90	210	108.00	187
52.00	102	71.05	137	87.00	307	109.05	969
56.90	284	72.05	157	88.95	9	110.00	552
57.95	99	72.95	120	91.95	176	111.00	75
59.00	355	74.00	134	92.95	482	112.15	164
61.75	210	76.05	333	96.05	266	113.00	199
62.90	1602	77.05	1533	97.95	399	115.00	216

Scan 1729 (33.649 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.00	184	131.00	278	148.05	191	167.00	98
116.95	412	133.95	53	148.95	281	167.80	101
117.95	144	136.00	183	149.95	32	171.80	50
121.00	17	137.00	304	152.05	32	172.95	259
122.05	31	138.10	11	152.95	52	175.05	76
124.05	177	139.00	289	154.00	156	177.05	108
125.95	71	140.10	48	154.95	242	177.75	204
127.05	2016	141.00	107	159.05	68	179.00	58
128.05	271	141.95	222	160.90	210	179.95	102
129.00	625	142.95	207	164.05	27	181.00	220
129.90	70	145.00	47	164.95	326	183.05	165

Scan 1729 (33.649 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
185.00	172	199.00	194	225.05	202	256.00	507
186.15	289	205.00	74	225.90	60	256.95	69
187.95	14	206.15	767	227.00	231	257.90	161
189.00	47	207.00	234	236.15	149	259.25	71
189.95	97	211.00	53	239.80	91	264.80	115
192.05	157	213.15	69	241.20	143	269.95	180
193.00	153	213.80	38	242.00	12	270.80	77
195.05	150	214.05	55	244.05	164	272.80	45
195.95	80	216.95	412	252.15	128	274.90	5823
197.05	146	218.05	92	253.00	148	275.90	856
198.05	484	223.95	357	255.00	2208	276.90	154

Scan 1729 (33.649 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
284.25	44						
286.40	74						

295.80	296
306.75	215
327.90	100
364.80	263
440.95	124
441.95	293
473.90	1635
475.00	267
475.90	219

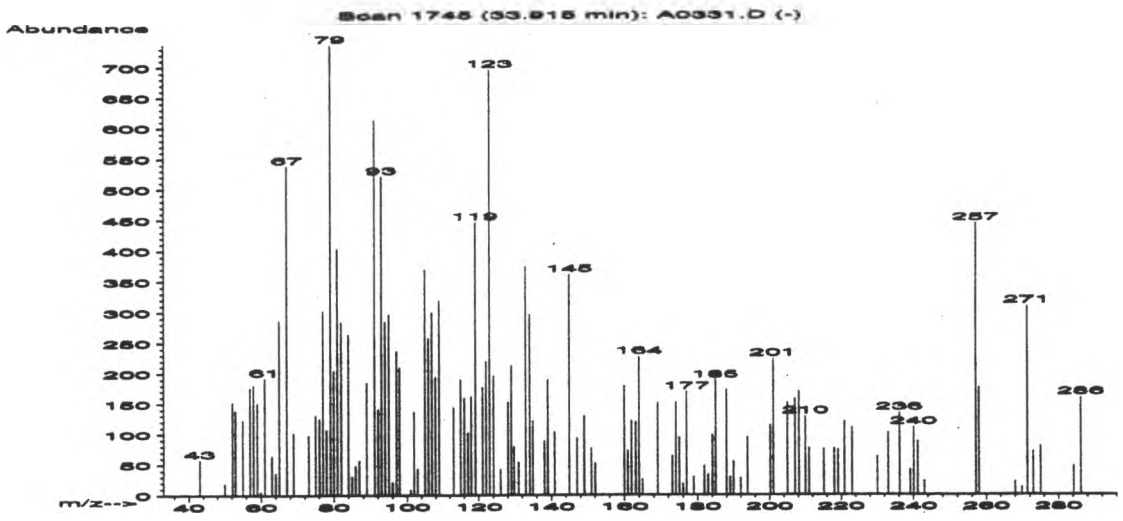
Scan 1729 (33.649 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	N-(4-CHLORO-3-(.ALPHA.,.ALPHA.,.ALPHA.-T	275	C11H5ClF3NO2	46
2.	4'-Nitro-(ortho-terphenyl)	275	C18H13NO2	38
3.	4-Nitro-(ortho-terphenyl)	275	C18H13NO2	38
4.	Naphtho[2,1-f]quinolin-2(1H)-one, 3,4,4a	275	C18H29NO	38
5.	1,2-Bis(4,6-diphenylpyrimidyl-1-oxy)etha	522	C34H26N4O2	38
6.	3-METHYL-4-NITRO-5-(4-NITRO)STYRYL-ISOXA	275	C12H9N3O5	37
7.	ANTI,ENDO-13-METHYL-12,14-DIOXO-13-AZATE	275	C15H17NO4	37
8.	Naphtho[2,1-f]quinolin-2(1H)-one, 3,4,4a	275	C18H29NO	32
9.	1,1':4',1''-Terphenyl, 4-nitro-	275	C18H13NO2	32
10.	Phenol, 4-[(2,4-dinitrophenyl)amino]-	275	C12H9N3O5	32
11.	ANTI,EXO-13-METHYL-12,14-DIOXO-13-AZATET	275	C15H17NO4	25
12.	SYN,EXO-13-METHYL-12,14-DIOXO-13-AZATETR	275	C15H17NO4	23
13.	2,2':6',2''-Terpyridine, 4,4',4''-trimet	275	C18H17N3	23
14.	1,1':4',1''-Terphenyl, 4-nitro-	275	C18H13NO2	23

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	000000-00-0	65219	49	100	1	87	43	20	0	46	8649
2.	*38	060366-38-3	65389	32	48	0	68	38	14	0	33	8563
3.	*38	060366-37-2	65388	31	35	0	70	38	14	2	35	8563
4.	*38	021171-75-5	65397	33	139	3	72	49	14	0	39	8566
5.	38	000000-00-0	109453	44	138	0	81	49	14	0	39	8575
6.	*37	078080-53-2	65232	33	17	1	97	42	13	8	35	8579
7.	*37	064776-94-9	65301	30	65	0	83	42	13	0	33	8575
8.	*32	021171-75-5	132419	39	93	1	68	49	9	6	31	8562
9.	*32	010355-53-0	65379	36	70	0	68	49	9	6	35	8563
10.	*32	000119-15-3	65231	35	74	1	96	49	9	6	32	8579
11.	*25	064813-04-3	65302	28	39	1	83	42	7	0	29	8575
12.	*23	064999-14-0	65303	29	68	1	83	49	6	0	29	8575
13.	*23	033354-75-5	65395	29	88	1	70	49	6	3	29	8566
14.	*23	010355-53-0	132417	32	112	1	67	49	6	0	26	8563

Peak 86



Scan 1745 (33.915 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	58	64.00	36	81.00	403	95.00	297
50.00	19	65.00	286	82.00	284	96.00	21
52.20	153	67.10	538	84.00	264	97.05	237
52.95	139	68.95	102	85.00	31	97.95	210
55.00	123	73.00	98	85.95	48	101.00	8
57.00	176	74.95	131	86.95	56	101.95	137
58.00	181	76.05	125	89.00	185	103.00	43
59.00	151	77.00	302	91.10	612	105.00	369
59.95	5	78.05	107	92.05	141	106.00	258
61.00	192	79.05	737	92.95	520	107.00	300
63.00	64	80.00	204	93.95	284	107.95	194

Scan 1745 (33.915 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.05	319	126.05	43	145.05	361	169.05	152
113.00	144	128.05	153	147.05	93	173.05	64
115.00	191	129.00	213	149.05	130	174.05	153
116.05	159	129.75	80	151.00	77	175.05	95
117.00	102	131.00	54	152.05	52	176.00	19
117.95	162	133.00	374	160.00	179	177.00	170
119.05	446	134.15	296	161.00	73	179.00	30
121.05	177	135.00	122	161.90	122	181.90	48
122.00	220	138.15	89	163.10	120	182.95	34
123.05	695	139.00	190	164.00	228	184.15	98
124.05	196	140.95	104	165.00	26	185.00	189

Scan 1745 (33.915 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
188.00	173	211.00	77	241.20	88		
189.05	30	215.20	75	243.00	23		
189.95	55	218.05	77	257.10	444		
192.00	28	219.15	74	258.00	177		
193.80	95	220.95	121	267.95	22		
200.20	115	223.05	111	269.80	12		
201.05	224	230.00	63	271.30	310		
205.00	151	233.00	102	272.95	71		
207.00	158	236.15	135	275.00	80		
208.15	171	239.05	42	284.15	47		
210.00	129	240.05	111	286.15	160		

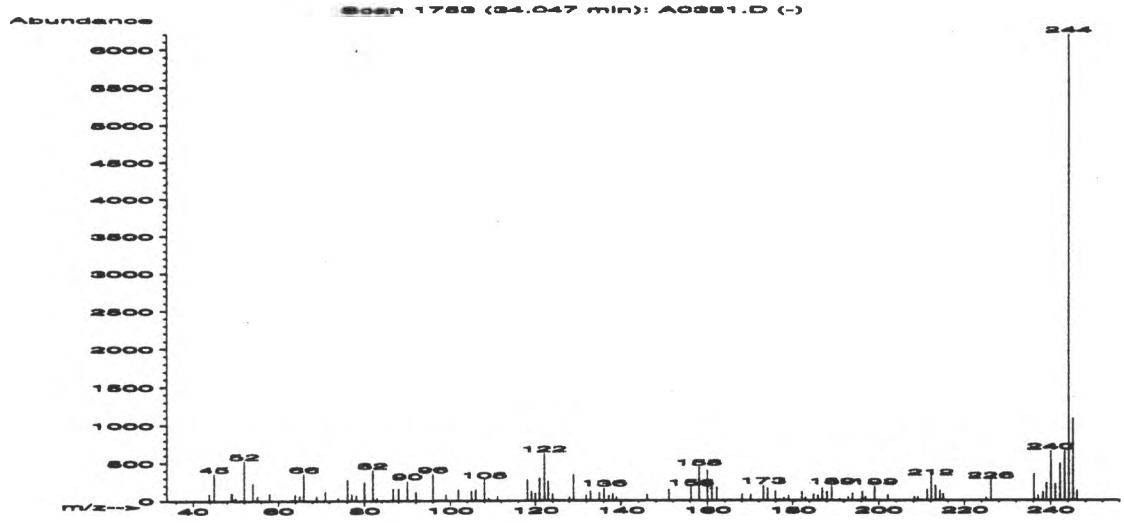
Scan 1745 (33.915 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 4-nitroso-	123	C6H5NO2	38
2.	Benzenesulfenic acid, methyl-	140	C7H8OS	32
3.	3-Hepten-1-yne, (E)-	94	C7H10	18
4.	Azocine, 2-methoxy-8-methyl-	149	C9H11NO	16
5.	4-exo-Bromobicyclp[3.2.0]hept-2-en-7-one	186	C7H7BrO	14
6.	4-exo-Bromobicyclp[3.2.0]hept-2-en-6-one	186	C7H7BrO	14
7.	Methyl-(endo-tricyclo[2.2.0.0(2,6)]hex-3	110	C7H10O	14
8.	Benzene, (2-propenyloxy)-	134	C9H10O	10
9.	2-Propenoic acid, 3-[(phenylmethyl)thio]	208	C11H12O2S	10
10.	1,3-DIMETHYL-1-BENZYL-5-PHENYL-2-PYRAZOL	392	C18H21IN2	10
11.	cis- 2,3-DIMETHYL-1,1-DIFLUOROCYCLOPROPA	106	C5H8F2	10
12.	Cyclohexane, 2-propynylidene-	120	C9H12	10
13.	3-Hepten-1-yne, (Z)-	94	C7H10	10
14.	cis-(5-Vinyl-2-cyclopenten-1-yl)methyl-p	278	C15H18O3S	10
15.	trans-3-(1Z,3-Butadienyl)-4-vinyl-cyclop	146	C11H14	10
16.	cis-3-(1Z,3-Butadienyl)-4-vinyl-cyclopen	146	C11H14	10
17.	Benzenemethanol, 2-amino-	123	C7H9NO	9
18.	Sclareol	308	C20H36O2	9
19.	Benzene, 1-azido-4-methyl-	133	C7H7N3	8
20.	Benzene, 1-azido-4-methyl-	133	C7H7N3	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	000104-91-6	4532	34	58	0	63	50	14	5	38	6882
2.	32	072347-63-8	9091	43	62	1	80	50	9	7	35	6870
3.	*18	000764-58-9	482	33	66	0	63	66	3	19	43	2619
4.	16	027153-33-9	12311	46	67	1	40	58	3	0	31	3768
5.	14	087973-94-2	28140	45	6	0	69	66	2	16	41	2619
6.	14	087973-93-1	28139	45	6	0	69	66	2	16	41	2619
7.	14	000000-00-0	2210	44	68	1	93	66	2	20	38	2619
8.	10	001746-13-0	7398	43	70	3	181	66	1	0	37	3176
9.	*10	077611-66-6	38274	43	88	1	56	61	1	6	27	3187
10.	10	000000-00-0	96427	46	113	3	127	66	1	0	37	2619
11.	10	000694-20-2	1744	45	68	1	64	66	1	0	37	2619
12.	10	002806-45-3	4153	47	78	1	75	66	1	0	31	2619
13.	*10	000764-57-8	481	40	70	1	91	66	1	0	33	2619
14.	10	090542-08-8	66309	44	27	1	70	66	1	0	37	2619
15.	10	084926-62-5	11488	47	68	1	80	66	1	0	31	2619
16.	10	084899-26-3	11487	47	68	1	80	66	1	0	31	2619
17.	* 9	005344-90-1	120313	39	77	1	103	79	1	0	35	6785
18.	9	000515-03-7	133720	45	162	3	96	73	1	0	34	7718
19.	* 8	002101-86-2	121456	31	97	3	125	66	1	0	26	2619
20.	* 8	002101-86-2	121455	28	87	3	137	66	1	0	26	2619

Peak 87



Scan 1753 (34.047 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.85	89	65.00	58	83.00	32	109.00	29
44.95	358	66.00	351	86.75	156	111.10	60
48.95	100	69.00	59	88.00	154	118.05	272
49.20	99	71.00	119	90.00	255	119.05	127
49.95	36	73.95	33	92.00	116	119.95	97
51.95	522	75.00	7	95.95	348	120.95	302
54.00	232	76.05	280	99.00	81	122.05	617
55.05	58	77.05	89	101.95	147	122.95	252
57.90	94	78.05	67	105.00	128	124.00	88
62.95	5	80.00	247	106.00	143	128.00	41
63.95	80	82.00	403	108.00	274	129.00	341

Scan 1753 (34.047 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.95	71	160.00	402	179.00	69	196.20	113
133.00	127	161.00	269	182.15	113	197.00	48
135.00	101	162.15	175	183.00	38	199.05	183
136.10	168	164.95	2	184.95	79	202.05	71
137.15	69	168.05	86	186.00	66	208.15	49
138.15	93	170.05	77	187.00	161	209.00	46
139.00	48	173.05	195	188.00	116	211.15	141
146.00	80	174.05	165	189.15	188	212.15	310
151.00	143	175.95	123	190.95	22	213.15	197
156.15	173	176.95	14	193.00	41	214.20	134
158.00	439	177.95	35	193.95	95	214.95	86

Scan 1753 (34.047 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
225.05	33	245.20	1083				
226.15	265	246.05	130				
236.15	347						
237.15	67						
238.15	112						
239.05	225						
240.05	650						
241.05	212						
242.20	484						
243.20	646						
244.20	6201						

Scan 1753 (34.047 min): A0331.D

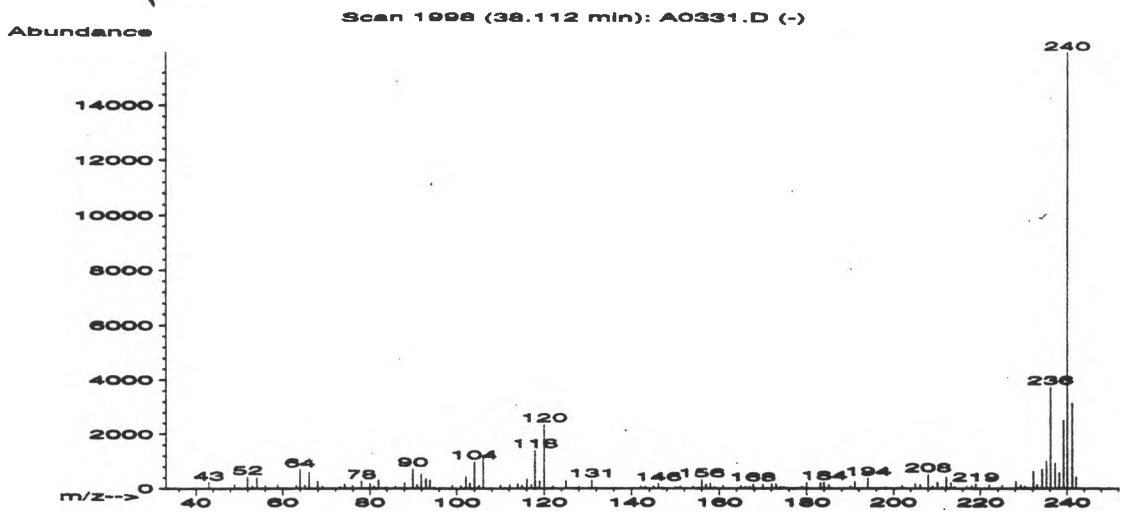
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ferrocene, (3-hydroxypropyl)-	244	C13H16FeO	76
2.	Benzene, 1,1',1''-methylidynetris-	244	C19H16	59
3.	1,4-Cyclohexadiene, 6-methylene-3,3-diph	244	C19H16	53
4.	Ferrocene, 1-(1-hydroxyethyl)-3-methyl-	244	C13H16FeO	42
5.	2-PROPENOIC ACID, 2-CYANO-3-(4-DIMETHYLA	244	C14H16N2O2	42
6.	Benzene, 1,1',1''-methylidynetris-	244	C19H16	42
7.	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimet	244	C14H16N2O2	42
8.	10-HYDROXY-7-METHYL-2H,9H-BENZO[1,2-B:5,	244	C13H8O5	40
9.	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimet	244	C14H16N2O2	40
10.	9H-Xanthen-9-one, 1,3,8-trihydroxy-	244	C13H8O5	40
11.	2-DIPHENYLMETHYLPYRIDINE	245	C18H15N	38
12.	1-(P-METHOXYPHENYL)-3-(2-THIENYL)-2-PROP	244	C14H12O2S	36
13.	6-Deoxyhemigossypol	244	C15H16O3	36
14.	1,2,3,4-Phenazinetetrol	244	C12H8N2O4	36
15.	1H-Pyrrolo[2,3-b]pyridine, 3-iodo-	244	C7H5IN2	36
16.	[1,1'-Biphenyl]-4,4'-diamine, 3,3'-dimet	244	C14H16N2O2	36
17.	(5-(2)H)1,3-DIMETHYL-(5,10-DIHYDRO)-5-DE	243	C13H12DN3O2	36
18.	2-DIPHENYLMETHYLPYRIDINE	245	C18H15N	34
19.	4,5,5-TRIETHYL-1,2-DIHYDRO-2,3-DIMETHYL-	273	C16H28BNSi	33
20.	Pregn-4-ene-3,20-dione, 16-methyl-, (16.	328	C22H32O2	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*76	012093-88-8	54017	64	63	2	99	21	45	0	64	9863
2.	*59	000519-73-3	131038	35	81	2	69	22	33	0	39	9778
3.	*53	018636-59-4	54298	35	73	1	80	28	28	11	40	9507
4.	*42	012289-11-1	54018	35	69	2	98	29	17	8	35	9837
5.	*42	001886-52-8	54113	38	103	2	71	28	17	0	33	9840
6.	*42	000519-73-3	131035	47	54	1	83	29	17	2	37	9771
7.	*42	000119-90-4	131022	36	107	3	99	28	17	0	35	9833
8.	*40	067406-85-3	53987	29	64	0	87	35	16	6	35	9823
9.	*40	020325-40-0	54096	35	62	0	96	35	16	0	35	9836
10.	*40	006052-93-3	53986	34	83	3	99	31	16	0	35	9816
11.	38	003678-70-4	131050	33	109	2	89	24	14	0	21	9044
12.	*36	000000-00-0	54055	35	81	2	71	29	12	0	27	9837
13.	*36	055824-28-7	54172	32	129	2	74	29	12	0	29	9801
14.	*36	025187-21-7	53956	30	130	2	99	28	12	0	29	9827
15.	*36	023616-57-1	53812	30	68	1	99	29	12	0	27	9798
16.	*36	000119-90-4	54095	32	109	2	83	26	12	0	26	9853
17.	*36	000000-00-0	53669	31	132	2	68	29	12	0	26	8025
18.	34	003678-70-4	54490	34	99	1	81	28	11	0	13	8893
19.	33	000000-00-0	64652	44	65	1	82	33	10	2	23	9793
20.	28	001922-34-5	82435	43	82	2	85	36	8	8	29	9788

Peak 80

Compounds from Proctor and Gamble A0331.D



Scan 1998 (38.112 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	223	65.00	110	82.00	309	96.05	8
43.95	12	66.00	601	83.95	27	96.95	15
48.95	141	67.95	252	85.95	68	99.05	117
49.90	19	69.05	80	87.00	17	100.95	90
51.95	424	73.00	55	88.05	203	102.05	436
53.05	84	74.05	154	90.00	712	102.95	204
54.05	393	75.95	101	91.00	130	104.00	982
56.00	96	78.00	268	91.95	523	105.00	110
58.90	140	79.05	8	93.05	365	106.00	1116
63.00	104	80.00	173	93.95	316	108.00	9
63.90	690	81.00	76	95.00	25	110.00	122

Scan 1998 (38.112 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.05	21	128.05	68	154.00	50	170.00	151
112.15	138	131.00	315	154.95	20	172.05	156
114.00	184	135.95	35	156.00	327	173.05	156
115.00	110	140.95	7	157.00	152	174.05	56
116.10	351	142.00	67	158.00	185	174.95	44
117.15	135	143.05	62	159.05	49	178.90	78
117.95	1398	144.95	92	160.95	100	180.00	210
118.95	278	146.05	188	165.00	106	183.15	217
120.05	2353	147.05	32	166.00	56	184.00	227
122.00	77	150.00	41	167.00	49	185.10	142
125.05	281	151.05	67	167.80	176	189.95	92

Scan 1998 (38.112 min): A0331.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
191.00	256	210.10	216	228.15	272	239.15	2502
194.05	380	211.15	48	229.15	123	240.05	15950
197.05	18	212.15	422	230.15	83	241.20	3144
198.20	37	213.15	204	231.05	21	242.05	416
199.20	15	214.05	66	232.15	639		
202.00	97	216.95	69	233.05	133		
205.00	169	218.05	87	234.15	709		
206.10	139	218.95	173	235.15	998		
207.00	14	221.05	21	236.15	3732		
208.00	519	222.05	142	237.15	935		
209.00	75	225.05	101	238.20	589		

Compounds from Proctor and Gamble A0331.D

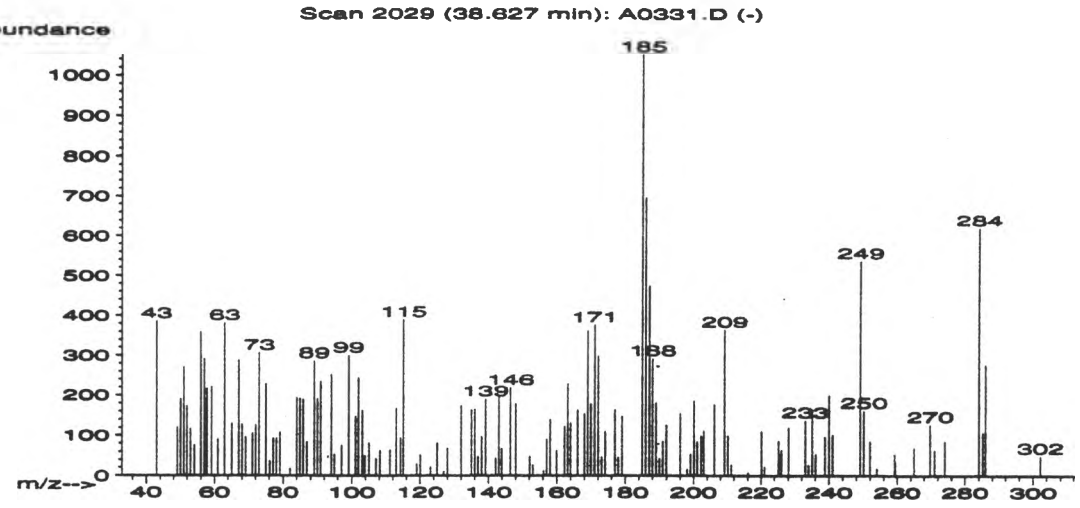
Scan 1998 (38.112 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	[1]Benzothieno[4,5-b][1]benzothiophene	240	C14H8S2	58
2.	[1]Benzothieno[3,2-b][1]benzothiophene	240	C14H8S2	53
3.	6,6-DIPHENYL-D5-2,4-PENTADIENYLIDENE-1	230	C18H4D10	53
4.	[1,1'-Biphenyl]-4,4'-diamine, 3,3',5,5'-	240	C16H20N2	50
5.	s-Triazolo[1,5-a]pyridine, 6-nitro-2-phe	240	C12H8N4O2	47
6.	Benzo[b]selenophene-3-carboxylic acid, 2	240	C10H8O2Se	45
7.	Iron, (.eta.5-2,4-cyclopentadien-1-yl)[(	240	C14H16Fe	42
8.	[1,1'-Biphenyl]-4,4'-diamine, N,N,N',N'-	240	C16H20N2	42
9.	9,10-Anthracenedione, 1,8-dihydroxy-	240	C14H8O4	42
10.	(+-)-Costaclavine	240	C16H20N2	40
11.	Naphtho[2,1-b:7,8-b']difuran, 1,2,9,10-t	240	C16H16O2	40
12.	Benzene, 1,1'-(1,2-ethenediyl)bis[4-meth	240	C16H16O2	40
13.	1,3,4-Thiadiazole, 2,3-dihydro-3,5-diphe	240	C14H12N2S	38
14.	2-Propen-1-one, 1-(2-hydroxyphenyl)-3-(4	240	C15H12O3	38
15.	4H-Naphtho[1,2-b]pyran-4-one, 5-methoxy-	240	C15H12O3	36
16.	1,9-(1'-ETHYLIDENEETHYLENE)DIAMANTANE	240	C18H24	28
17.	N-PHENYL(F)(3,5)PYRAZOLOPHANE	240	C16H20N2	28
18.	9,10-Anthracenedione, 1,5-dihydroxy-	240	C14H8O4	28

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	055134-02-6	52513	50	77	3	78	27	32	0	44	9658
2.	*53	000248-70-4	52514	40	63	2	99	30	28	7	40	9631
3.	*53	055530-35-3	48587	35	86	3	89	27	28	20	40	8461
4.	*50	054827-17-7	52756	48	78	2	76	33	25	0	39	9401
5.	*47	031040-17-2	52374	39	56	3	92	39	20	3	38	9485
6.	*45	026526-42-1	52305	34	146	2	99	24	19	0	30	7899
7.	*42	033039-67-7	52557	35	105	3	99	27	17	0	30	9716
8.	*42	000366-29-0	52739	39	101	2	97	27	17	0	33	9694
9.	*42	000117-10-2	130798	34	98	1	99	30	17	0	35	9634
10.	*40	074644-95-4	52753	31	36	1	99	33	16	6	35	9587
11.	*40	068873-21-2	52715	29	63	1	74	33	16	5	34	9584
12.	*40	004705-34-4	52693	30	79	0	98	33	16	0	33	9592
13.	*38	036358-07-3	52551	28	64	2	99	39	14	1	30	9418
14.	*38	013323-66-5	52609	36	102	3	92	36	14	0	35	8560
15.	*36	032454-43-6	52625	32	137	3	99	30	12	0	27	9351
16.	*28	059297-01-7	52800	29	79	2	95	39	8	0	27	9494
17.	*28	037072-11-0	52743	28	104	1	99	39	8	0	29	9494
18.	*28	000117-12-4	52512	28	108	3	66	36	8	0	27	9650

Peak 89



Scan 2029 (38.627 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	386	60.90	90	77.05	93	94.05	251
49.05	120	62.95	381	78.05	92	95.05	53
49.95	191	65.00	129	79.05	108	97.05	75
50.95	271	67.05	288	82.00	18	99.05	299
51.90	174	68.00	128	84.00	193	101.05	147
52.95	117	69.05	96	84.95	192	101.95	243
54.00	76	71.05	105	85.90	189	103.05	162
55.90	359	71.95	126	86.95	83	103.80	50
57.00	291	73.05	306	89.10	285	105.00	81
57.75	216	75.05	228	90.00	190	107.00	42
59.00	222	76.10	36	91.00	234	108.15	62

Scan 2029 (38.627 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.10	64	135.00	163	152.05	48	168.95	361
113.00	168	136.00	165	153.00	26	169.95	178
114.25	94	137.00	47	156.10	11	170.95	375
115.05	389	138.00	96	157.10	89	172.05	297
119.00	29	139.10	190	158.15	139	173.05	46
120.05	52	141.05	2	159.90	62	174.05	109
123.05	21	142.05	43	162.15	122	177.00	163
125.00	81	143.05	194	163.15	229	177.95	45
127.00	10	143.90	67	164.00	130	179.05	147
128.00	68	146.45	218	166.05	163	185.00	1051
132.00	174	148.05	178	168.05	153	186.00	695

Scan 2029 (38.627 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
187.00	473	202.15	98	226.00	63	251.90	84
188.00	291	203.00	111	228.15	120	254.00	18
189.00	180	206.15	176	233.00	137	259.15	53
189.95	41	209.15	364	234.00	25	259.50	34
190.95	84	210.15	99	235.05	163	264.95	68
191.95	125	211.20	27	236.05	53	269.70	126
196.05	154	214.75	1	238.80	96	271.00	62
198.05	15	216.15	8	240.05	199	274.05	84
199.05	53	220.05	110	241.05	101	284.00	620
200.05	185	221.05	21	249.05	535	285.15	106
201.05	83	225.15	86	250.15	161	286.00	275

Scan 2029 (38.627 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
302.15	48						

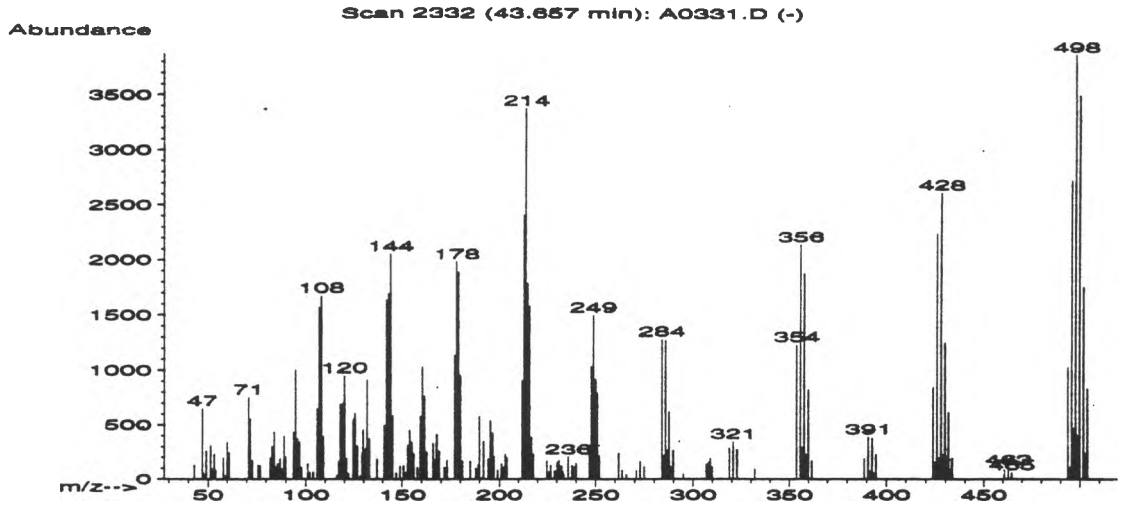
Scan 2029 (38.627 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	5-Ethylidene-10-hydroximino-10,11-dihydr	249	C17H15NO	27
2.	4-CHLOROTHIENO(2,3-B)PYRIDINE 7-OXIDE	185	C7H4ClNOS	27
3.	4(1H)-Quinazolinone, 2,3-dihydro-3-(2-pr	186	C11H10N2O	27
4.	3,5-DIMETHYL-1-BENZYLPYRAZOLE	186	C12H14N2	16
5.	Benzaldehyde, 4-bromo-	184	C7H5BrO	16
6.	E-2-BENZYLIDENE CYCLOHEXANONE	186	C13H14O	16
7.	3-(3',6',6'-TRIMETHYLCYCLOHEX-1'-EN-1'-Y	200	C12H21Cl	16
8.	6-HYDROXY-7-CHLOROBENZO-2,1,3-THIADIAZON	186	C6H3ClN2OS	14
9.	9,10-Dihydro-9-methyl-9,10-([1',7']-tric	284	C22H20	12
10.	Estra-1,3,5(10)-trien-17-one, 3-methoxy-	284	C19H24O2	12
11.	1,2-Azaborolidine, 1-(1,1-dimethylethyl)	201	C13H20BN	10
12.	Benzene, 1,1'-thiobis-	186	C12H10S	10
13.	4-CHLOROPHENOL-TRIMETHYL-SILYL-ETHER	200	C9H13ClOSi	10
14.	Ethene, 1,2-dibromo-	184	C2H2Br2	10
15.	1-(Phenyl-d(5)-1-d-2-phenylethylene	180	C14H6D6	9
16.	3-BROMO-P-CRESOL	186	C7H7BrO	9
17.	Cyclohexanone, 2-(phenylmethylene)-	186	C13H14O	9
18.	4-CHLOROPHENOL-TRIMETHYL-SILYL-ETHER	200	C9H13ClOSi	9
19.	5,10-DIHYDROXY-2-METHOXY-7-METHYL-1,4-AN	284	C16H12O5	9
20.	Phenol, phenoxy-, mono(1-methylethoxy) d	244	C15H16O3	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*27	070449-97-7	56073	39	102	0	36	58	8	0	39	3325
2.	*27	025557-54-4	27879	34	112	1	99	59	8	0	39	7266
3.	*27	031084-13-6	28443	33	95	2	97	60	8	0	39	7679
4.	*16	001134-81-2	28560	38	87	2	71	60	3	0	33	7728
5.	16	001122-91-4	27172	46	81	1	75	60	3	6	35	7648
6.	*16	001467-15-8	127417	35	87	1	71	60	3	18	36	7673
7.	*16	054344-72-8	34778	38	74	2	91	59	3	0	35	7300
8.	*14	029105-93-9	28115	55	60	1	48	67	2	0	40	6110
9.	*12	078365-71-6	68699	32	23	0	40	64	2	0	33	3755
10.	*12	017748-69-5	68617	34	110	1	44	64	2	7	34	6024
11.	*10	072443-04-0	35190	44	77	3	219	75	1	0	40	5874
12.	*10	000139-66-2	127396	33	77	0	56	78	1	0	41	7278
13.	*10	000000-00-0	128360	34	93	1	53	79	1	0	39	7381
14.	*10	000540-49-8	127121	33	89	0	57	78	1	0	41	5084
15.	* 9	000000-00-0	25892	26	102	0	59	79	1	6	35	6488
16.	* 9	000000-00-0	28132	33	81	2	69	75	1	11	36	4879
17.	* 9	005682-83-7	28588	42	96	1	61	71	1	0	35	7668
18.	* 9	000000-00-0	34526	32	93	0	59	78	1	11	35	7497
19.	* 9	074815-58-0	68402	46	121	1	41	78	1	0	35	7007
20.	9	072361-23-0	54147	38	100	0	66	71	1	0	33	5617

Peak 90



Scan 2332 (43.657 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	131	61.00	243	85.90	141	102.00	62
46.95	653	69.00	9	87.00	189	103.95	65
47.70	56	70.95	754	87.90	93	105.90	653
48.95	264	71.80	556	89.15	398	106.90	1565
51.05	315	73.00	170	89.90	204	108.00	1671
51.95	95	75.95	130	93.95	437	109.00	393
53.05	228	77.00	123	94.95	1003	116.05	38
53.95	84	82.00	194	95.95	373	116.95	160
57.90	198	82.95	303	96.95	345	117.85	687
58.95	31	84.00	434	97.95	105	118.95	697
60.00	344	85.05	111	101.00	141	119.95	948

Scan 2332 (43.657 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
121.05	189	137.00	184	154.00	450	167.80	412
122.00	52	140.80	497	155.00	342	168.95	260
124.45	547	141.95	1628	155.75	231	171.80	107
125.30	605	142.95	1688	156.00	227	173.05	176
126.55	305	143.95	2045	158.00	108	176.95	1132
128.00	30	144.95	583	159.40	578	177.90	1972
129.15	237	147.00	58	160.40	1025	178.90	1876
129.75	453	149.00	119	161.40	759	179.90	948
130.95	281	150.80	124	162.65	251	180.95	160
131.90	911	152.05	63	165.95	330	185.15	166
133.00	372	153.00	315	166.80	176	187.90	98

Scan 2332 (43.657 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
189.05	133	203.00	229	226.90	126	239.10	111
189.80	579	203.90	196	228.90	74	239.95	143
190.85	9	211.90	904	229.20	6	246.80	230
191.95	348	212.90	2391	230.25	156	247.80	1029
194.30	185	213.80	3357	231.15	170	248.80	1490
195.30	539	214.80	1778	232.50	119	249.95	912
196.45	423	215.80	1571	233.15	67	250.90	787
197.15	207	216.80	383	233.50	40	251.90	208
199.05	82	217.80	230	235.90	204	261.75	237
201.05	140	224.95	166	237.05	9	263.70	82
201.95	107	226.00	65	237.80	127	265.80	44

Scan 2332 (43.657 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
270.80	81	306.75	136	357.75	1862	424.75	156

Compounds from Proctor and Gamble A0331.D

272.80	165	307.90	153	358.75	224	425.65	2231
274.75	113	308.75	190	359.80	814	426.75	194
283.90	1273	309.75	110	361.70	165	427.75	2599
284.90	218	318.80	288	388.70	188	428.65	220
285.75	1264	320.80	345	390.70	387	429.75	1244
286.70	268	322.80	273	391.80	74	430.75	195
287.70	618	332.00	96	392.70	374	431.65	610
288.70	111	353.75	1224	393.80	54	432.80	87
289.80	268	355.75	2127	394.70	223	433.45	187
294.95	49	356.90	289	423.65	843	460.70	88

Scan 2332 (43.657 min): A0331.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
460.95	85	502.75	231				
462.80	106	503.65	829				
464.70	60						
493.65	1026						
494.65	110						
495.65	2717						
496.65	468						
497.65	3875						
498.65	405						
499.65	3495						
501.65	1750						

Compounds from Proctor and Gamble A0331.D

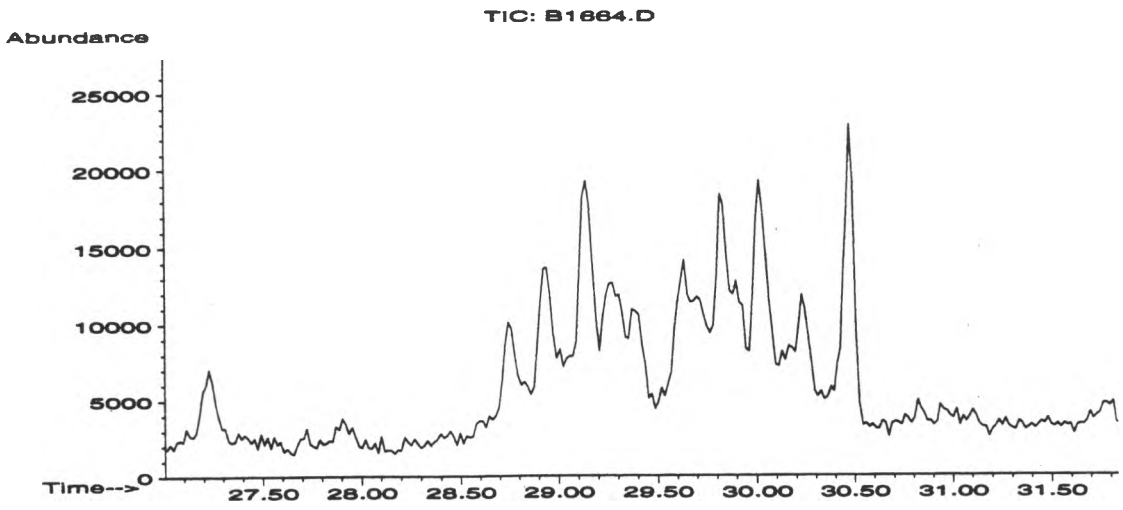
Scan 2332 (43.657 min): A0331.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Perchlorobiphenyl	494	C12Cl10	38
2.	4-HYDROXY NONACHLORODIPHENYL ETHER	492	C12HCl9O2	27
3.	1,3,6-Tribromobenzo[1,2-c:3,4-c]dithioph	424	C10H3Br3S2	11
4.	2,3,9,10-TETRACHLORO-BENZO[1,2-B:4,5-B']	426	C18H6Cl4O4	7
5.	2-HYDROXY NONACHLORODIPHENYL	492	C12HCl9O2	6

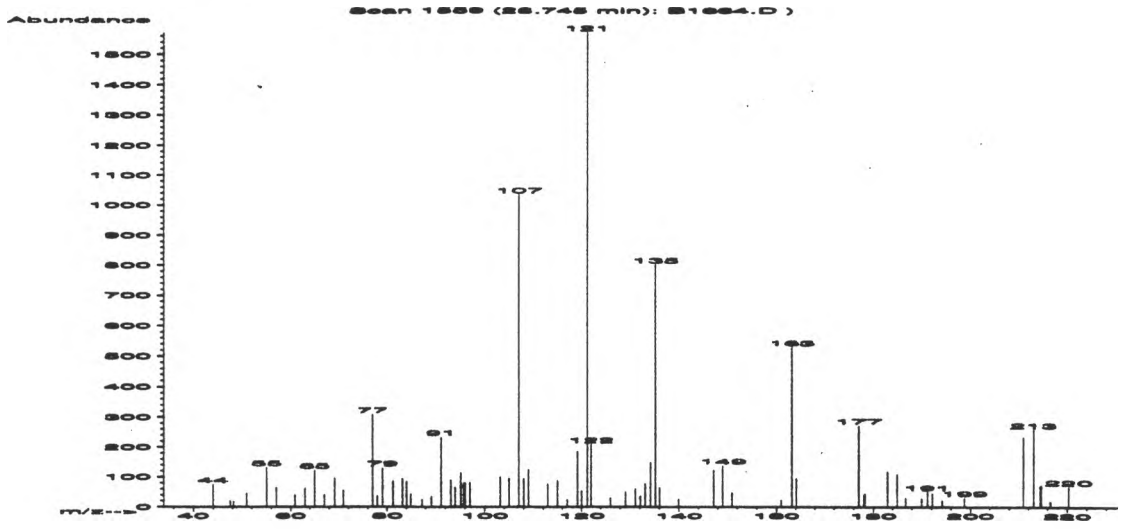
	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	002051-24-3	136934	147	101	3	80	65	14	40	66	6105
2.	*27	021567-21-5	108295	62	185	2	70	59	8	0	39	8166
3.	*11	088687-02-9	101380	52	60	2	212	78	2	0	46	4546
4.	* 7	068641-78-1	101680	28	134	2	49	77	1	0	27	4677
5.	* 6	035245-80-8	108294	39	217	2	60	70	1	0	12	7532

Nonylphenols in Weldwood B1664.D



Nonylphenol Isomers

Nonylphenol Isomer [1]



Scan 1559 (28.745 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	75	70.90	55	93.15	90	113.00	77
47.55	21	77.05	309	94.00	66	115.00	89
48.20	18	78.05	35	95.15	114	117.00	25
50.95	45	79.05	130	95.75	78	119.15	185
55.05	131	81.20	87	96.00	81	120.00	54
57.05	65	83.20	94	97.00	81	121.15	1570
60.90	40	84.05	85	103.20	100	122.00	208
63.00	62	84.95	43	105.05	97	126.05	30
65.00	122	87.25	25	107.05	1034	129.05	49
67.00	41	89.15	35	108.05	94	131.05	60
69.15	96	91.15	233	109.05	124	132.05	36

Scan 1559 (28.745 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.05	78	177.05	271	210.95	233		
134.20	149	178.05	40	213.05	257		
135.20	801	178.30	44	214.45	70		
136.05	64	182.95	118	214.70	73		
139.90	26	184.95	108	216.50	18		
147.15	122	186.70	29	220.25	68		
149.00	137	189.95	29				
150.95	46	191.15	49				
160.95	23	192.15	44				
163.20	527	194.15	23				
164.15	95	198.75	30				

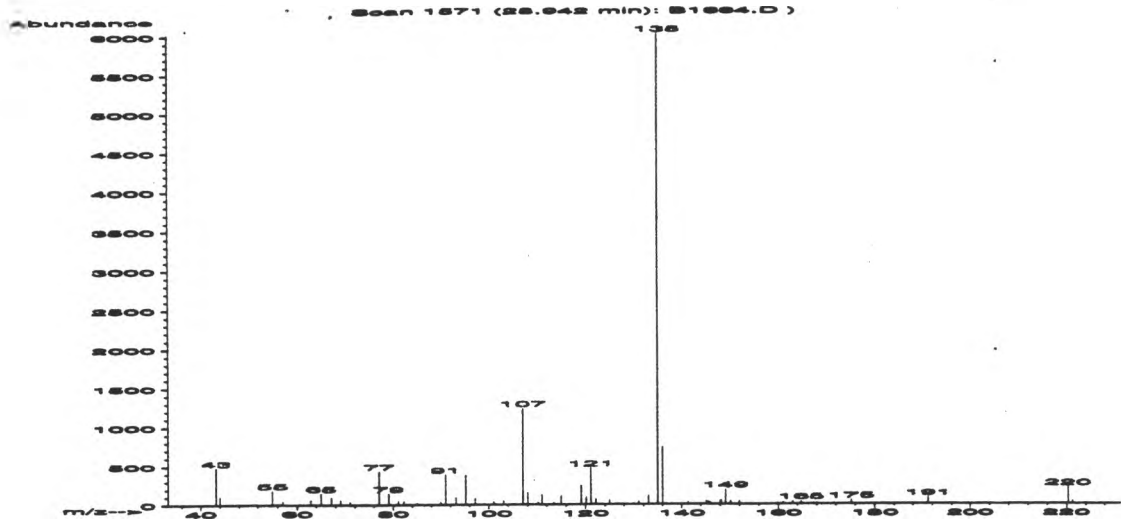
Scan 1559 (28.745 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	NONYLPHENOL ISOMER	220	C15H24O	98
2.	Phenol, 4-nonyl-	220	C15H24O	27
3.	Phenol, nonyl-	220	C15H24O	27
4.	CIS-ANTI-CIS-TRICYCLO[7.3.0.0(2,6)]DODEC	164	C12H20	27
5.	Acetamide, N-methyl-N-(4-methylphenyl)-	163	C10H13NO	27
6.	Benzenamine, 3,4-dimethyl-	121	C8H11N	25
7.	Benzenamine, 2,4-dimethyl-	121	C8H11N	25
8.	Benzenamine, 2,4-dimethyl-	121	C8H11N	25
9.	Benzenamine, 3,5-dimethyl-	121	C8H11N	25
10.	Benzenamine, 3,4-dimethyl-	121	C8H11N	25
11.	Benzenamine, 2,6-dimethyl-	121	C8H11N	22
12.	Benzenamine, 2,6-dimethyl-	121	C8H11N	22
13.	Benzeneacetic acid, .alpha.-methoxy-, me	180	C10H12O3	22
14.	Benzenamine, 3,5-dimethyl-	121	C8H11N	22
15.	Benzene, (1-methoxyethyl)-	136	C9H12O	22
16.	Phenol, 4-ethyl-3-methyl-	136	C9H12O	22
17.	2-Oxazolidinone, 4-phenyl-5-p-tolyl-, tr	253	C16H15NO2	22
18.	Phenol, 4-(1-methylethyl)-	136	C9H12O	22
19.	Benzenamine, 3,4-dimethyl-	121	C8H11N	22
20.	NONYLPHENOL ISOMER	220	C15H24O	11

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*98	000000-00-0	129726	119	10	0	93	10	79	51	98	9819
2.	*27	000104-40-5	129723	34	74	2	128	60	8	11	40	7013
3.	27	025154-52-3	43894	47	51	0	47	60	8	12	41	7850
4.	*27	030159-15-0	18777	50	47	2	86	60	8	21	39	8065
5.	*27	000612-03-3	18074	42	56	0	78	56	8	0	39	7630
6.	*25	000095-64-7	120095	50	52	0	71	63	7	0	46	7607
7.	*25	000095-68-1	4239	44	54	0	88	63	7	0	44	7483
8.	*25	000095-68-1	120090	45	57	0	81	63	7	0	44	7579
9.	*25	000108-69-0	4243	48	56	0	81	63	7	0	46	7556
10.	*25	000095-64-7	4242	51	51	0	79	63	7	0	46	7544
11.	*22	000087-62-7	120094	33	70	2	99	63	5	0	39	7587
12.	*22	000087-62-7	120092	39	59	0	91	63	5	0	39	7496
13.	22	056143-21-6	25496	47	12	0	80	65	5	16	41	7258
14.	*22	000108-69-0	120097	28	65	0	99	65	5	3	42	7502
15.	*22	004013-34-7	7961	45	47	1	91	64	5	0	39	7372
16.	22	001123-94-0	121905	45	43	2	98	63	5	0	39	7470
17.	22	032461-31-7	57728	43	74	2	92	63	5	0	39	7413
18.	*22	000099-89-8	7900	49	36	1	88	64	5	17	39	7427
19.	*22	000095-64-7	120096	40	63	0	75	63	5	0	39	7609
20.	*11	000000-00-0	43895	48	65	2	144	73	2	0	46	6237

Nonylphenol Isomer [2]



Scan 1571 (28.942 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.15	476	81.05	50	108.05	155	133.05	116
44.00	105	82.20	46	110.20	29	135.05	6023
54.95	187	84.95	23	111.05	131	136.05	739
57.05	51	89.90	34	113.50	21	141.40	30
62.90	64	91.00	390	115.00	111	145.15	45
65.00	150	93.15	91	119.15	245	145.50	29
67.15	96	95.15	384	120.15	92	145.90	26
69.00	65	97.15	82	121.15	469	148.00	47
71.00	43	100.95	33	122.15	73	148.25	47
77.05	430	103.05	57	124.95	51	149.15	191
79.05	148	107.05	1239	131.05	35	150.15	45

Scan 1571 (28.942 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.95	42						
161.05	28						
163.05	36						
164.75	37						
168.00	18						
175.15	52						
191.15	86						
220.25	211						
221.25	41						

Nonylphenol Isomers

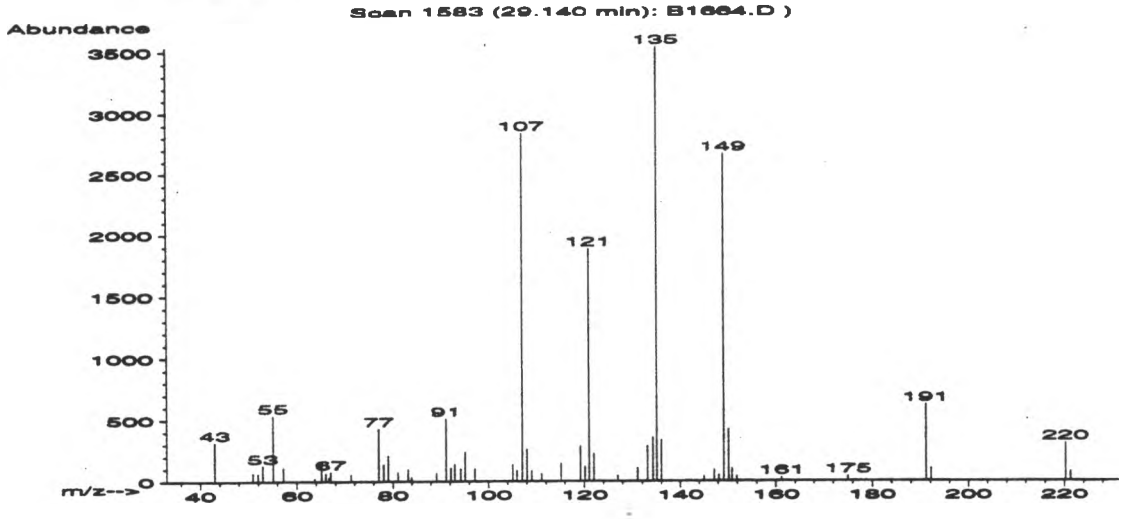
Scan 1571 (28.942 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	72
2.	OCTYL PHENOL ISOMER	206	C14H22O	72
3.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	64
4.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	64
5.	Phenol, 4-nonyl-	220	C15H24O	64
6.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	56
7.	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	50
8.	Ethanone, 1-(4-methoxyphenyl)-	150	C9H10O2	50
9.	6-METHOXY-3-METHYL-2-BENZOTHIAZOLINETHIO	211	C9H9NOS2	50
10.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	50
11.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	45
12.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	45
13.	NONYLPHENOL ISOMER	220	C15H24O	45
14.	Phenol, nonyl-	220	C15H24O	42
15.	NONYLPHENOL ISOMER	220	C15H24O	42
16.	Benzoic acid, 4-(bromomethyl)-	214	C8H7BrO2	39
17.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	39
18.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	37
19.	THYMYL ACETATE	192	C12H16O2	36
20.	Silane, trimethylphenyl-	150	C9H14Si	36

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	000098-54-4	123674	45	35	0	70	12	42	17	39	9866
2.	72	000000-00-0	37565	44	37	1	99	12	42	2	41	9944
3.	64	000140-66-9	128870	45	44	1	93	18	37	2	41	9937
4.	64	000140-66-9	128869	47	57	0	89	20	37	0	39	9936
5.	64	000104-40-5	129723	43	64	3	82	16	37	8	41	9441
6.	56	000585-34-2	123671	51	29	1	71	12	30	2	33	9907
7.	50	000080-46-6	125356	43	16	0	72	16	25	11	33	9934
8.	50	000100-06-1	123644	38	38	0	69	20	25	13	35	9912
9.	50	000000-00-0	39792	40	54	2	71	16	25	4	37	9933
10.	50	000089-83-8	123683	39	52	1	68	16	25	13	35	9950
11.	45	000499-75-2	123692	37	50	2	67	23	19	4	33	9954
12.	45	000499-75-2	123691	37	50	2	67	23	19	4	33	9954
13.	*45	000000-00-0	43895	55	56	3	85	23	19	0	35	9732
14.	*42	025154-52-3	43894	34	92	3	78	27	17	0	30	8912
15.	42	000000-00-0	129727	48	56	3	99	27	17	0	31	9811
16.	39	006232-88-8	40963	35	74	2	94	20	15	0	25	9928
17.	39	000499-75-2	123693	35	50	1	66	16	15	4	26	9951
18.	37	000098-54-4	123676	41	44	0	58	41	13	4	35	9886
19.	36	000000-00-0	30864	35	62	1	82	29	12	0	25	9785
20.	36	000768-32-1	12691	33	44	0	86	30	12	0	25	9735

Nonylphenol Isomer [3]



Scan 1583 (29.140 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	318	71.25	56	94.15	101	120.15	119
50.95	69	77.05	426	95.15	235	121.00	1884
51.95	61	78.05	136	97.15	104	122.00	225
52.95	126	79.05	207	105.05	137	126.95	44
55.05	534	81.05	70	105.95	88	131.05	106
57.20	110	83.20	95	107.05	2832	133.05	286
63.75	25	83.95	33	108.05	261	134.20	354
65.15	165	89.15	66	109.05	85	135.05	3534
66.00	66	91.15	507	111.05	62	136.05	335
66.65	30	92.15	108	115.15	142	145.00	38
67.00	76	93.00	140	119.15	284	147.15	87

Scan 1583 (29.140 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.15	50						
149.15	2665						
150.15	418						
150.95	99						
151.95	36						
161.20	28						
175.00	40						
191.15	619						
192.15	102						
220.25	305						
221.25	73						

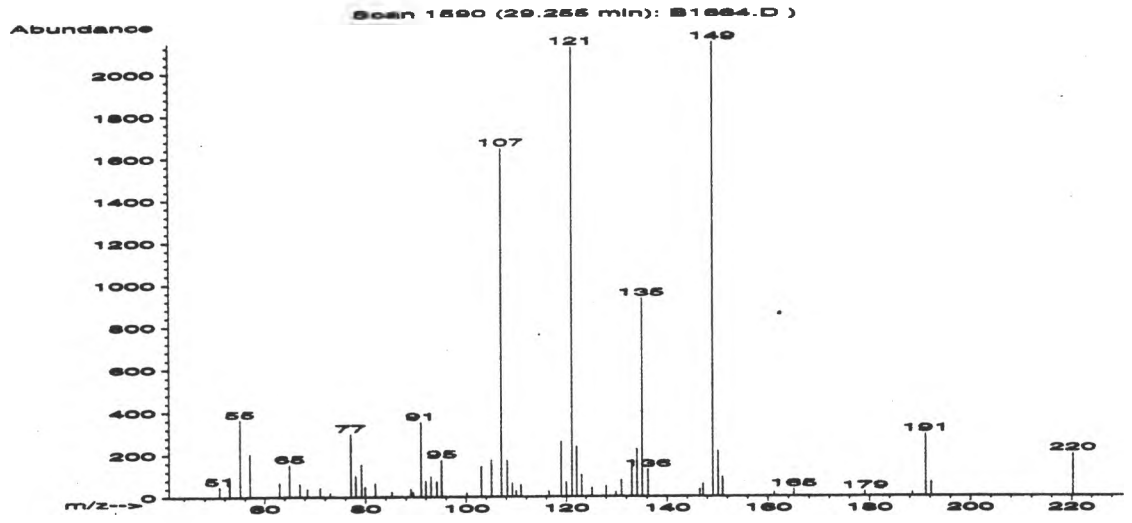
Scan 1583 (29.140 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, nonyl-	220	C15H24O	86
2.	Phenol, 4-nonyl-	220	C15H24O	76
3.	Phenol, 4-nonyl-	220	C15H24O	62
4.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	60
5.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	46
6.	NONYLPHENOL ISOMER	220	C15H24O	46
7.	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	43
8.	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	43
9.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	35
10.	Phenol, 4-(2-methylpropyl)-	150	C10H14O	35
11.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	35
12.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	35
13.	ACETOPHENONE, 2'-METHOXY-	150	C9H10O2	22
14.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	22
15.	2-ETHYLFORMANILIDE	149	C9H11NO	22
16.	1-(2,3,5,6-Tetramethylpyridyl)-2-propano	191	C12H17NO	22
17.	Phenol, 4-propyl-	136	C9H12O	18
18.	3-(4-Methoxyphenyl)heptan-4-one	220	C14H20O2	14
19.	2-AMINO-3,5-DIMETHYL-BENZALDEHYDE	149	C9H11NO	14
20.	1,2-Benzenedicarboxylic acid, bis(1-meth	250	C14H18O4	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	025154-52-3	43894	88	42	1	127	30	53	0	89	9640
2.	*76	000104-40-5	43893	77	53	1	95	24	45	0	81	9666
3.	*62	000104-40-5	129723	72	49	1	179	30	36	0	53	9185
4.	*60	000088-18-6	12725	63	31	0	86	39	35	28	64	7850
5.	*46	000103-89-9	123491	53	38	0	70	42	20	21	46	6495
6.	*46	000000-00-0	43895	69	47	2	188	53	20	0	76	8833
7.	*43	000537-92-8	123489	59	33	0	72	42	18	12	41	6489
8.	*43	000120-66-1	123488	58	34	1	75	42	18	8	41	6607
9.	*35	000088-18-6	123668	35	33	1	71	52	11	5	40	7852
10.	*35	004167-74-2	12724	65	22	0	67	67	11	0	64	5334
11.	*35	000499-75-2	123692	46	49	0	89	54	11	18	40	7320
12.	*35	000499-75-2	123691	46	49	0	89	54	11	18	40	7319
13.	*22	000000-00-0	12617	36	48	1	76	64	5	14	40	6427
14.	22	000499-75-2	123689	39	49	1	97	64	5	21	43	6767
15.	*22	002860-30-2	12323	36	63	0	54	61	5	0	41	6234
16.	*22	070660-34-3	30432	51	22	0	63	65	5	20	40	4774
17.	*18	000645-56-7	121890	48	32	1	64	69	3	16	44	5014
18.	*14	084736-57-2	43743	35	14	1	75	68	2	0	41	5756
19.	*14	070128-12-0	12297	43	44	1	54	66	2	0	40	5805
20.	14	000605-45-8	131296	47	64	0	58	67	2	0	39	4865

Nonylphenol Isomer [4]



Scan 1590 (29.255 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
50.95	49	78.05	99	95.15	175	120.00	71
52.95	96	79.20	153	100.20	18	121.15	2116
55.05	363	79.95	48	103.05	143	122.15	235
57.05	204	81.95	66	105.05	174	123.15	102
63.00	68	85.20	24	107.05	1644	125.20	41
65.00	153	89.00	37	108.20	172	128.05	51
67.00	62	89.40	23	109.20	68	129.95	22
68.50	38	91.00	352	109.95	29	131.05	78
71.00	44	92.00	76	110.95	59	133.05	170
72.95	19	93.00	98	116.50	28	134.05	223
77.05	296	94.15	74	119.00	260	135.05	932

Scan 1590 (29.255 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
136.20	129	192.25	68				
146.50	35	220.25	199				
147.15	59						
149.15	2139						
150.15	212						
151.05	91						
161.20	19						
165.00	33						
179.05	23						
188.55	18						
191.15	292						

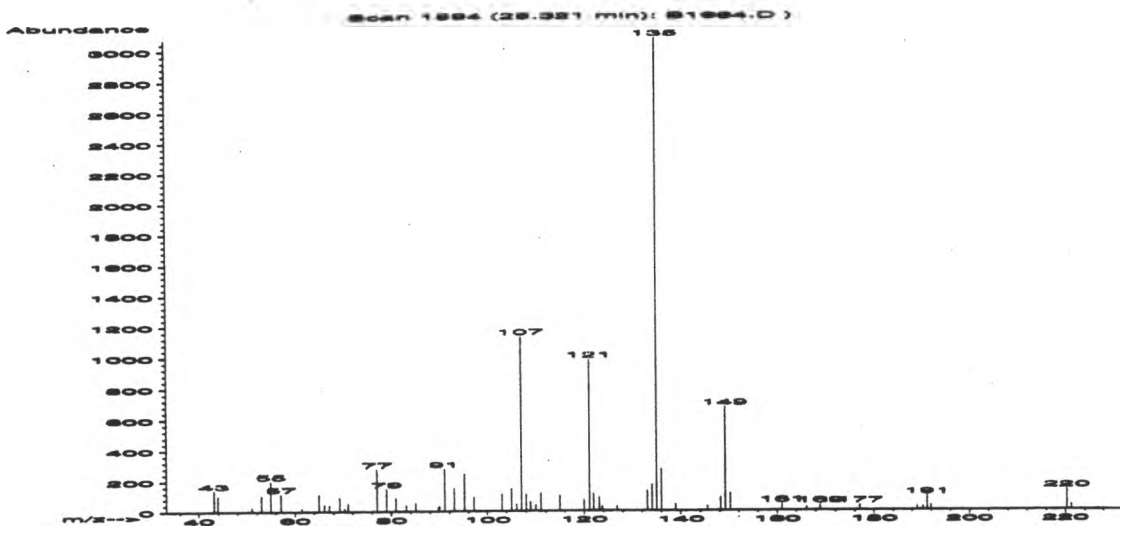
Scan 1590 (29.255 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	NONYLPHENOL ISOMER	220	C15H24O	46
2.	Phenol, nonyl-	220	C15H24O	46
3.	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	43
4.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	43
5.	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	38
6.	Phenol, 2,4,6-trimethyl-	136	C9H12O	27
7.	1,4-Cyclohexadiene, 3,3,6,6-tetramethyl-	136	C10H16	18
8.	1,2-Benzenedicarboxylic acid, bis(1-meth	250	C14H18O4	14
9.	2-METHYL-6-PROPYLPHENOL	150	C10H14O	14
10.	4-METHYL-2-PROPYLPHENOL	150	C10H14O	14
11.	Benzenemethanol, 4-(1,1-dimethylethyl)-	164	C11H16O	14
12.	5-methyl-7-amino-S-triazolo(1,5-A)pyrimi	149	C6H7N5	14
13.	Benzene, 1-methoxy-4-octyl-	220	C15H24O	14
14.	Phenol, 2-(1-methylpropyl)-	150	C10H14O	14
15.	Anisole, p-octyl-	220	C15H24O	14
16.	Phenol, 4-butyl-	150	C10H14O	11
17.	Phenol, 3-ethyl-5-methyl-	136	C9H12O	11
18.	Benzenamine, 2,6-dimethyl-	121	C8H11N	10
19.	Benzenemethanol, .alpha.-ethyl-	136	C9H12O	10
20.	Phenol, 4-ethyl-3-methyl-	136	C9H12O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	000000-00-0	129728	52	64	1	85	42	20	9	44	8642
2.	*46	025154-52-3	129725	52	64	1	85	42	20	9	44	8642
3.	*43	000537-92-8	123489	59	31	0	89	50	18	18	47	6575
4.	*43	000103-89-9	123490	36	50	0	90	50	18	18	43	6584
5.	*38	000120-66-1	123488	52	37	1	89	50	14	2	41	6762
6.	27	000527-60-6	7910	44	55	1	92	60	8	0	39	6568
7.	*18	002223-54-3	8097	55	37	2	98	69	3	0	49	6000
8.	14	000605-45-8	131296	43	69	0	88	69	2	0	39	6156
9.	*14	003520-52-3	12888	48	35	1	98	69	2	12	39	6066
10.	*14	004074-46-8	12899	50	35	0	70	69	2	4	41	6032
11.	14	000877-65-6	18589	43	46	0	67	69	2	0	39	6646
12.	*14	033376-96-4	12206	34	30	1	88	67	2	1	40	6038
13.	*14	067698-82-2	44072	34	69	0	72	68	2	0	41	6067
14.	*14	000089-72-5	123662	34	56	2	98	66	2	19	40	6463
15.	*14	003307-19-5	43906	35	58	0	77	69	2	0	41	6037
16.	*11	001638-22-8	12720	44	38	0	57	72	2	0	44	4883
17.	*11	000698-71-5	121904	50	35	0	82	71	2	19	47	6367
18.	*10	000087-62-7	120092	33	65	0	77	71	1	0	41	6157
19.	*10	000093-54-9	121919	43	48	1	66	76	1	0	40	4565
20.	*10	001123-94-0	121905	45	35	0	72	72	1	5	40	6095

Nonylphenol Isomer [5]



Scan 1594 (29.321 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.15	137	70.25	19	95.15	239	120.00	69
43.90	101	71.00	52	97.15	90	121.15	980
50.95	25	77.05	274	103.05	109	122.00	109
52.95	102	79.05	144	105.05	145	123.15	85
54.95	197	80.95	86	106.05	43	123.75	26
57.05	113	83.05	39	107.05	1130	126.80	31
61.40	23	85.05	54	108.05	108	133.05	130
65.00	108	89.65	28	108.95	61	134.05	169
66.15	43	89.90	33	110.05	40	135.05	3069
67.15	39	91.00	276	111.05	116	136.05	270
69.25	91	93.00	149	115.00	98	139.00	41

Scan 1594 (29.321 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
145.50	30	191.90	31				
148.15	86	220.25	133				
149.15	673	221.25	34				
150.15	111						
161.05	40						
166.15	22						
168.90	36						
177.05	34						
189.05	26						
190.25	23						
191.15	91						

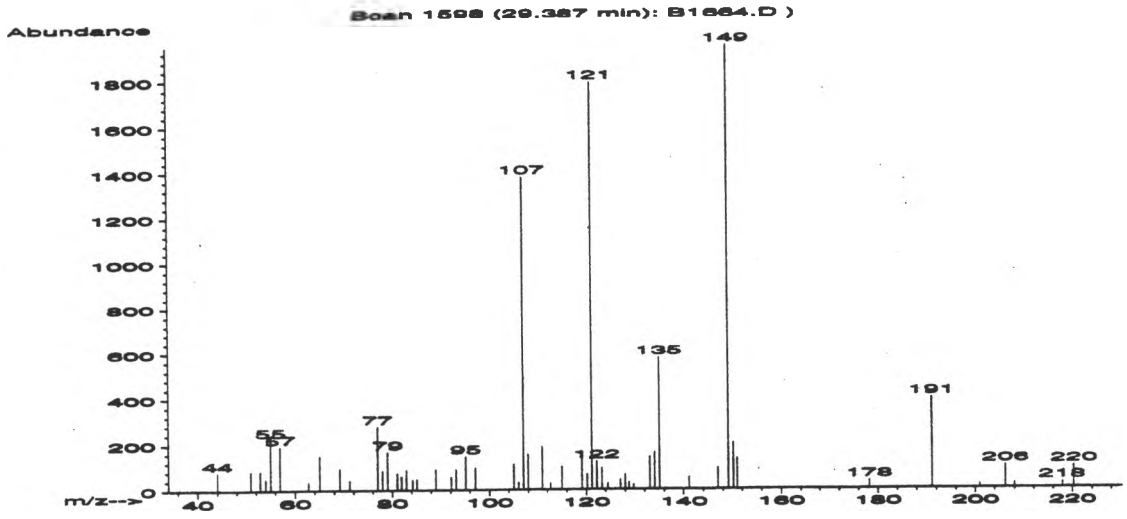
Scan 1594 (29.321 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	NONYLPHENOL ISOMER	220	C15H24O	95
2.	Phenol, nonyl-	220	C15H24O	91
3.	Phenol, 4-nonyl-	220	C15H24O	72
4.	Phenol, 4-nonyl-	220	C15H24O	70
5.	NONYLPHENOL ISOMER	220	C15H24O	64
6.	Phenol, 4-dodecyl-	262	C18H30O	64
7.	Phenol, 4-nonyl-	220	C15H24O	56
8.	Phenol, diethyl-	150	C10H14O	50
9.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	50
10.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	50
11.	Bicyclo[2.2.1]hept-2-en-7-ol, 7-(4-metho	216	C14H16O2	47
12.	Benzene, 1-(1,3-dimethyl-3-butenyl)-4-me	190	C13H18O	43
13.	2-NONYLPHENOL	220	C15H24O	43
14.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	42
15.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	40
16.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	40
17.	Benzeneacetonitrile, 3-fluoro-	135	C8H6FN	40
18.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	38
19.	Benzothiazole	135	C7H5NS	38
20.	Benzothiazole	135	C7H5NS	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	000000-00-0	43895	85	26	0	80	4	74	0	94	9988
2.	*91	025154-52-3	43894	81	45	1	71	13	62	0	84	9848
3.	*72	000104-40-5	129723	63	56	2	99	18	42	0	44	9949
4.	*70	000104-40-5	43893	74	55	1	50	29	41	0	81	9815
5.	64	000000-00-0	129727	77	25	0	92	24	37	0	45	9774
6.	64	000104-43-8	60617	65	48	1	68	8	37	1	37	9920
7.	56	000104-40-5	129724	74	41	1	66	11	30	5	37	9883
8.	50	026967-65-7	12731	41	45	1	67	32	25	10	39	9050
9.	*50	000499-75-2	123689	40	43	1	86	31	25	10	39	9178
10.	50	000140-66-9	128869	47	51	1	83	32	25	16	38	9562
11.	47	013118-72-4	42085	43	57	0	97	39	20	0	39	9246
12.	43	074672-05-2	30132	45	43	1	80	44	18	9	38	9164
13.	*43	000136-83-4	44071	56	54	0	57	44	18	12	40	9750
14.	42	000585-34-2	123672	43	55	2	79	29	17	0	34	9486
15.	40	000585-34-2	12726	44	48	2	81	31	16	0	35	9464
16.	40	000098-54-4	123674	44	48	3	85	31	16	0	37	9620
17.	*40	000501-00-8	7538	41	60	1	69	31	16	0	33	8836
18.	*38	015816-45-2	7331	33	53	3	99	40	14	0	35	9176
19.	*38	000095-16-9	121697	38	40	1	97	39	14	2	35	9236
20.	*38	000095-16-9	121696	30	56	3	93	40	14	0	33	9174

Nonylphenol Isomer [6]



Scan 1598 (29.387 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	79	78.05	84	97.15	95	122.15	122
50.95	82	79.05	166	105.05	113	123.25	96
52.95	84	81.05	73	106.05	32	124.40	27
53.95	48	81.95	59	107.05	1377	127.05	43
55.05	224	82.95	87	108.05	155	128.05	65
56.95	192	84.20	44	110.95	189	128.80	31
62.75	36	85.05	47	112.65	28	129.80	21
65.00	149	89.00	90	115.00	100	133.05	142
69.15	94	92.15	57	119.15	145	134.05	163
71.15	43	93.15	89	120.15	65	135.05	577
77.05	277	95.15	146	121.15	1789	141.15	52

Scan 1598 (29.387 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
147.00	93						
149.15	1948						
150.15	202						
150.95	134						
178.20	34						
191.15	397						
200.90	18						
206.20	100						
208.05	22						
217.90	25						
220.25	97						

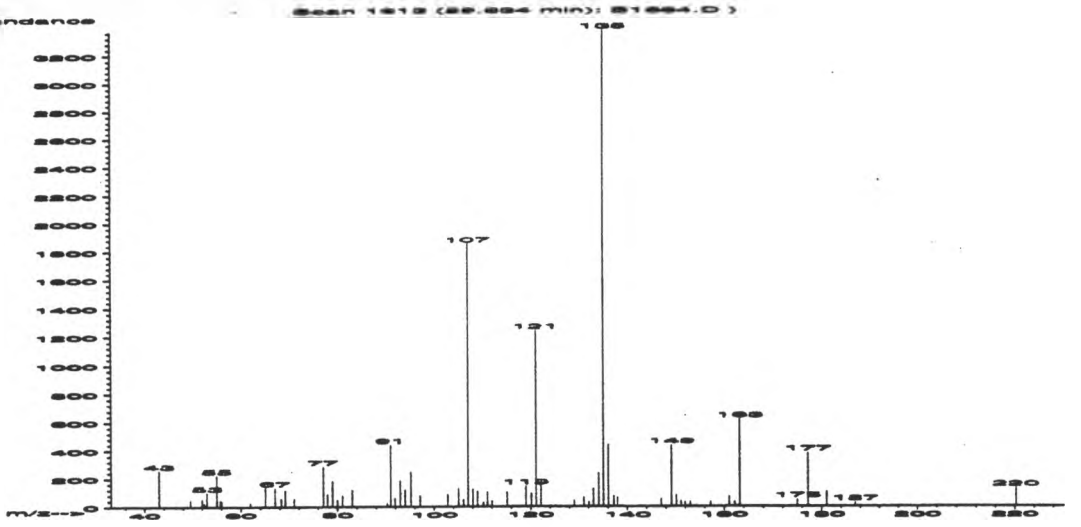
Scan 1598 (29.387 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-(1,1-dimethylethyl)-5-methyl-	164	C11H16O	47
2.	Tricyclo[3.3.1.1(3,7)]decanone, 4-iodo-,	276	C10H13IO	38
3.	2-Ethoxy-1-(3'-pyridyl)ethylene	149	C9H11NO	38
4.	NONYLPHENOL ISOMER	220	C15H24O	38
5.	Phenol, nonyl-	220	C15H24O	38
6.	NONYLPHENOL ISOMER	220	C15H24O	38
7.	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	35
8.	1,3-CYCLOHEXADIENE, 1,3,5,5,6,6-HEXAMETH	164	C12H20	32
9.	Silane, chlorotripropyl-	192	C9H21ClSi	32
10.	CYCLOHEXYL PENTYL PHTHALATE	318	C19H26O4	22
11.	Phenol, 4-(1-methylpropyl)-	150	C10H14O	22
12.	Phenol, 4-(2-methylpropyl)-	150	C10H14O	11
13.	Phenol, 4-butyl-	150	C10H14O	11
14.	1-Methoxy-4-(oxiran-2-yl)methylbenzene	164	C10H12O2	10
15.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	10
16.	5-methyl-7-amino-S-triazolo(1,5-A)pyrimi	149	C6H7N5	10
17.	Benzenemethanol, .alpha.-methyl-.alpha.-	228	C16H20O	10
18.	Benzene, 1-methoxy-4-(2-phenylethyl)-	212	C15H16O	10
19.	Benzenamine, N,2-dimethyl-	121	C8H11N	10
20.	Benzenamine, 3,5-dimethyl-	121	C8H11N	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	47	000088-60-8	125360	43	54	0	90	37	20	0	39	8566
2.	38	056781-86-3	65457	43	71	2	82	37	14	0	34	8585
3.	*38	000000-00-0	12273	33	57	1	93	37	14	0	35	8604
4.	38	000000-00-0	129728	43	63	0	81	49	14	2	41	8822
5.	38	025154-52-3	129725	43	63	0	81	49	14	2	41	8822
6.	38	000000-00-0	129726	57	56	0	79	47	14	16	43	7775
7.	*35	000120-66-1	123488	42	47	1	93	52	11	5	38	6855
8.	32	000000-00-0	18723	39	60	3	88	49	9	8	37	8022
9.	32	000995-25-5	30652	49	65	2	74	48	9	6	33	9431
10.	22	000000-00-0	79548	45	66	1	87	65	5	9	38	6530
11.	*22	000099-71-8	123664	33	55	0	68	64	5	0	41	6313
12.	*11	004167-74-2	12724	45	42	0	61	78	2	0	44	4978
13.	*11	001638-22-8	12720	53	29	0	53	80	2	0	49	4800
14.	10	000000-00-0	18455	39	54	0	66	68	1	0	33	5950
15.	10	000131-16-8	131293	39	67	0	99	66	1	0	33	6511
16.	*10	033376-96-4	12206	32	37	2	99	66	1	0	33	6369
17.	10	074685-13-5	47816	47	56	1	71	70	1	0	37	5810
18.	10	014310-21-5	40601	38	61	0	71	70	1	0	33	5810
19.	*10	000611-21-2	120087	33	69	1	70	68	1	0	35	6173
20.	*10	000108-69-0	4243	29	74	0	67	68	1	0	33	6092

Nonylphenol Isomer [7]



Scan 1613 (29.634 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	256	68.25	58	91.90	58	110.30	29
49.55	47	69.15	117	93.00	184	111.05	103
51.95	53	71.00	56	94.00	119	112.00	39
52.45	25	77.05	285	95.15	245	115.15	103
53.05	100	77.95	87	97.15	77	119.00	144
55.05	223	79.05	184	102.80	85	120.15	92
55.80	42	80.05	47	105.05	130	121.15	1238
56.05	40	81.05	77	106.05	49	122.15	156
61.90	28	83.05	120	107.05	1852	129.05	43
65.00	136	90.25	21	108.05	125	131.05	65
67.00	134	91.00	437	109.05	108	132.05	31

Scan 1613 (29.634 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
132.95	127	153.05	32				
134.05	238	157.20	31				
135.05	3370	161.05	69				
136.05	440	162.20	32				
137.20	75	163.20	617				
138.00	63	175.00	48				
147.00	55	177.20	381				
149.15	434	181.05	103				
150.15	78	186.95	26				
151.05	40	220.25	128				
151.95	31						

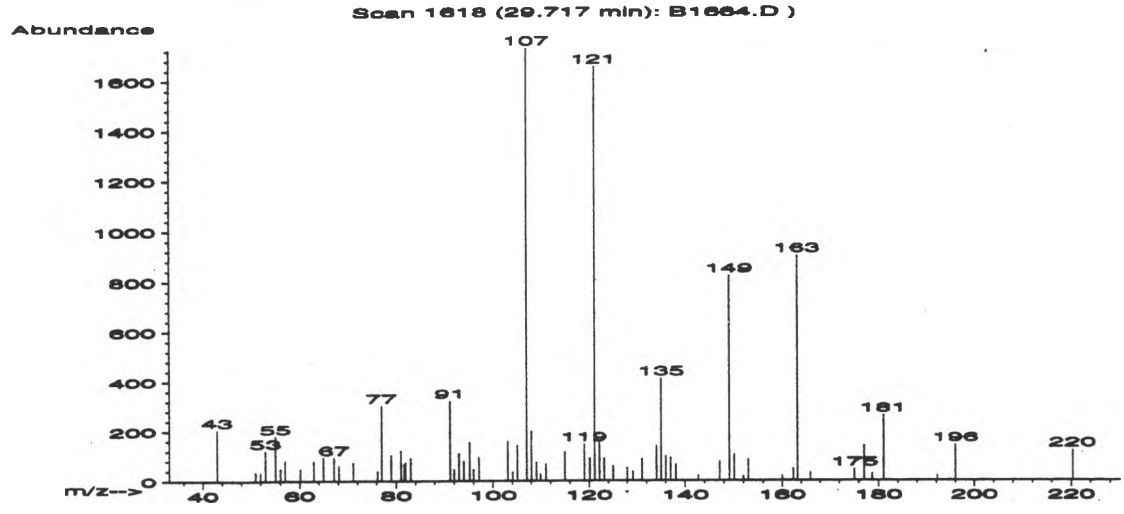
Scan 1613 (29.634 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, nonyl-	220	C15H24O	90
2.	Phenol, 4-nonyl-	220	C15H24O	87
3.	NONYLPHENOL ISOMER	220	C15H24O	74
4.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	64
5.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	59
6.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	58
7.	Phenol, 4,4'-(1,2-diethyl-1,2-ethanediyl	270	C18H22O2	53
8.	Phenol, 2,3,5,6-tetramethyl-	150	C10H14O	47
9.	1-Ethyleneaminoadamantane	177	C12H19N	47
10.	Phenol, diethyl-	150	C10H14O	43
11.	Thieno[3,2-c]pyridine	135	C7H5NS	43
12.	2-NONYLPHENOL	220	C15H24O	38
13.	ADAMANTANE, 1-BROMO-	214	C10H15Br	38
14.	2,3,4,6-Tetramethylpyridine	135	C9H13N	38
15.	NONYLPHENOL ISOMER	220	C15H24O	25
16.	Benzeneacetic acid, 4-hydroxy-	152	C8H8O3	11
17.	Phenol, 2-propyl-	136	C9H12O	11
18.	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	10
19.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	10
20.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	025154-52-3	43894	76	51	2	87	9	59	0	74	9634
2.	*87	000104-40-5	129723	78	41	1	82	15	54	37	74	9626
3.	*74	000000-00-0	43895	71	41	1	99	19	44	0	53	9686
4.	*64	000098-54-4	123676	51	37	2	99	25	37	16	45	9524
5.	59	000585-34-2	123671	52	36	2	98	25	33	3	38	9483
6.	*58	000098-54-4	123674	62	25	2	99	27	32	12	47	9552
7.	53	005635-50-7	63693	53	55	2	98	27	28	5	41	9725
8.	47	000527-35-5	12735	41	49	2	92	37	20	17	38	9088
9.	*47	000000-00-0	24322	34	43	2	94	38	20	0	41	9015
10.	*43	026967-65-7	12731	44	41	2	99	41	18	6	43	8828
11.	*43	000272-14-0	7534	35	62	3	69	45	18	0	39	8699
12.	*38	000136-83-4	44071	56	60	0	63	48	14	2	38	9766
13.	38	000000-00-0	129302	47	50	3	99	47	14	0	39	8838
14.	*38	020820-82-0	121733	33	50	3	74	50	14	0	39	7851
15.	25	000000-00-0	129727	75	30	2	142	65	7	0	45	9657
16.	*11	000156-38-7	13348	35	21	0	49	77	2	18	43	4658
17.	*11	000644-35-9	7895	44	32	0	37	72	2	0	44	4941
18.	*10	000120-66-1	123488	45	29	1	42	72	1	22	43	4654
19.	*10	000103-89-9	123491	42	33	0	37	72	1	17	38	4704
20.	*10	000103-89-9	123490	46	29	0	38	72	1	19	39	4704

Nonylphenol Isomer [8]



Scan 1618 (29.717 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	206	68.15	60	93.00	110	109.95	26
50.95	35	71.15	73	94.00	79	111.05	66
51.95	33	76.20	40	95.15	154	115.00	117
52.95	121	77.05	303	96.00	46	119.00	147
55.05	179	79.05	104	97.15	94	120.15	90
56.05	49	81.05	122	103.05	158	121.15	1654
56.95	81	81.70	67	104.05	36	122.15	157
60.15	48	81.95	74	105.05	141	123.15	89
62.90	80	83.05	91	107.05	1727	125.05	59
64.90	95	91.15	322	108.05	199	128.05	53
67.15	94	92.00	46	109.05	74	129.20	37

Scan 1618 (29.717 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.05	87	153.05	83	220.25	121		
134.05	140	160.05	19				
135.05	411	162.30	46				
136.05	97	163.20	901				
137.05	92	165.90	32				
138.15	64	175.15	45				
142.75	22	177.05	140				
147.15	76	178.70	27				
149.15	821	181.05	262				
150.15	105	192.25	20				
152.05	18	196.00	143				

Nonylphenol Isomers

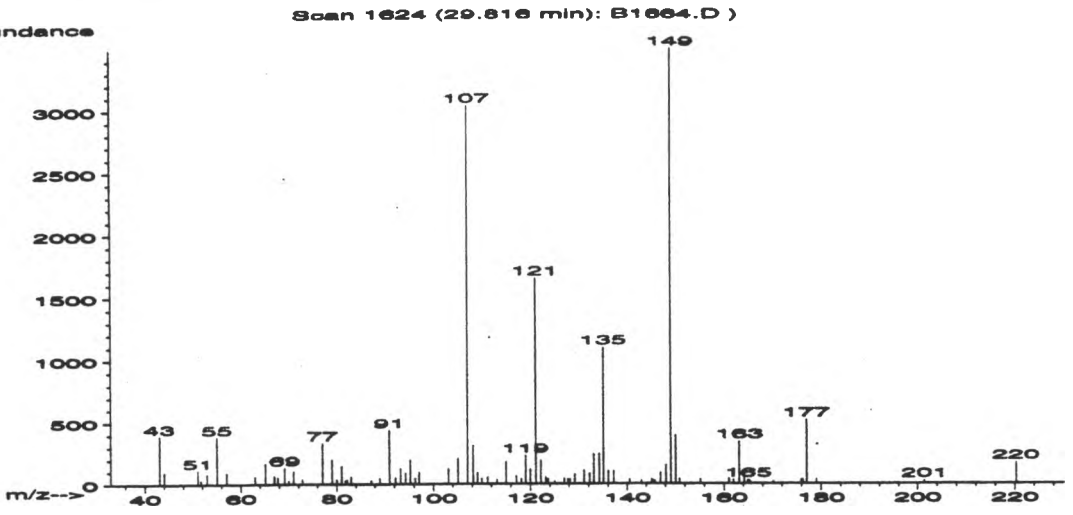
Scan 1618 (29.717 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	NONYLPHENOL ISOMER	220	C15H24O	58
2.	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	30
3.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	30
4.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	30
5.	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	30
6.	Thiocyanic acid, 4-oxotricyclo[3.3.1.1(3	207	C11H13NOS	27
7.	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	27
8.	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	27
9.	N-(P-TOLYL)-PROPIONIC ACID AMIDE	163	C10H13NO	27
10.	Phenol, 3,4-dimethyl-	122	C8H10O	22
11.	Benzeneacetic acid, 4-ethoxy-	180	C10H12O3	22
12.	2-METHYL-6-PROPYLPHENOL	150	C10H14O	18
13.	Phenol, 3-(1-methylethyl)-	136	C9H12O	18
14.	Benzeneacetic acid, .alpha.,4-dihydroxy-	196	C10H12O4	18
15.	Phenol, 4-ethyl-3-methyl-	136	C9H12O	18
16.	Phenol, 2-(1-methylethyl)-	136	C9H12O	14
17.	Phenol, 3-ethyl-	122	C8H10O	14
18.	Phenol, 4-(1-methylethyl)-	136	C9H12O	14
19.	TRIMETHYLSILYL-BUTADIYNE	122	C7H10Si	14
20.	Benzenemethanol, ar-ethyl-	136	C9H12O	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*58	000000-00-0	129726	62	68	2	84	30	32	13	45	8974
2.	*30	000120-66-1	123488	45	47	1	83	56	9	0	44	6996
3.	*30	000103-89-9	123490	52	40	1	90	56	9	0	46	6992
4.	*30	000103-89-9	123491	52	40	0	90	56	9	0	46	6992
5.	*30	000537-92-8	123489	44	42	0	99	56	9	0	44	6994
6.	27	056781-89-6	37896	45	72	2	66	56	8	0	39	6662
7.	*27	000537-92-8	12283	47	41	1	83	56	8	0	39	6989
8.	*27	000120-66-1	12282	35	61	2	99	56	8	0	41	6988
9.	*27	000000-00-0	18067	40	43	0	99	56	8	0	39	7054
10.	*22	000095-65-8	120224	52	30	1	95	65	5	21	41	6585
11.	22	004919-33-9	25491	46	43	1	67	63	5	23	41	6487
12.	*18	003520-52-3	12888	50	32	0	77	68	3	17	44	6294
13.	*18	000618-45-1	121897	43	45	2	95	68	3	20	47	6295
14.	*18	054845-39-5	32698	52	60	1	95	67	3	0	46	6444
15.	*18	001123-94-0	121905	49	33	0	76	69	3	17	44	6263
16.	14	000088-69-7	121893	42	45	2	81	69	2	2	39	6210
17.	14	000620-17-7	4388	43	46	2	99	68	2	0	39	6347
18.	*14	000099-89-8	7900	50	37	1	87	69	2	17	39	6229
19.	*14	000000-00-0	4378	46	39	1	95	66	2	22	43	6315
20.	*14	053957-34-9	7916	34	66	2	72	67	2	11	40	7193

Nonylphenol Isomer [9]



Scan 1624 (29.816 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	390	69.15	132	87.25	29	107.05	3036
44.00	98	70.00	25	89.00	49	108.20	316
51.05	112	71.00	104	91.00	438	109.05	92
51.70	28	72.80	35	92.15	53	109.95	45
52.95	82	77.05	333	93.15	128	111.20	57
55.05	382	79.05	200	94.15	91	113.15	36
57.05	93	80.05	37	95.15	196	115.00	180
63.00	61	81.05	147	96.15	52	117.15	68
65.15	165	81.80	29	97.00	99	118.15	40
67.00	70	82.20	34	103.05	125	119.00	232
67.75	53	83.05	60	105.05	209	120.00	119

Scan 1624 (29.816 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
121.15	1655	133.05	242	148.15	154	170.15	21
122.15	190	134.20	245	149.15	3493	175.90	30
123.15	58	135.05	1098	150.15	391	176.25	34
123.65	40	136.05	106	150.95	42	177.05	515
125.05	24	137.20	105	155.20	35	179.05	36
126.95	46	140.50	36	161.05	45	201.40	25
127.70	38	143.00	29	161.95	33	220.25	171
128.20	38	145.15	39	163.20	344		
129.20	77	145.50	28	164.15	87		
131.05	112	145.90	22	165.00	31		
132.20	85	147.00	92	165.40	23		

Nonylphenol Isomers

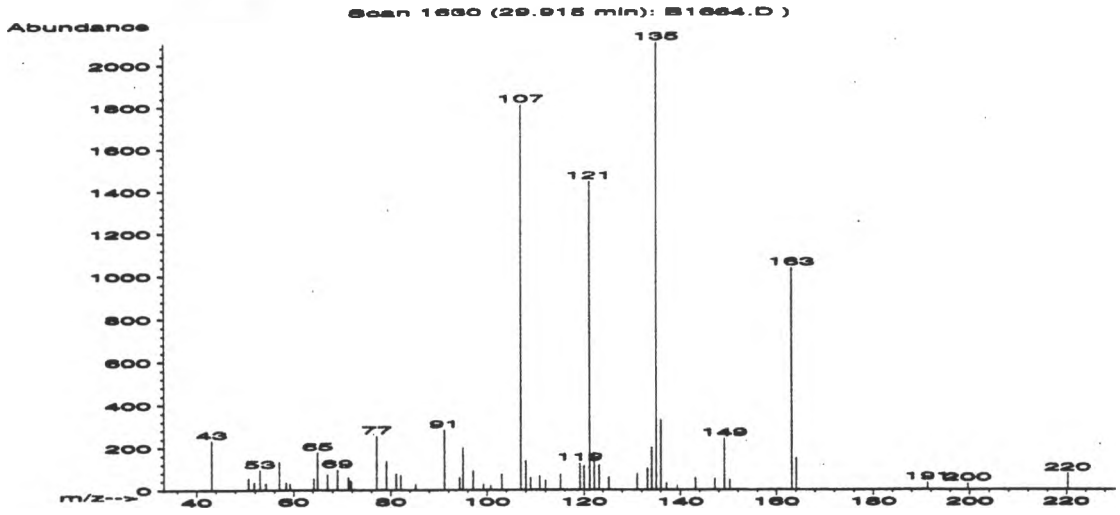
Scan 1624 (29.816 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, nonyl-	220	C15H24O	64
2.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	64
3.	NONYLPHENOL ISOMER	220	C15H24O	64
4.	Acetamide, N-(3-methylphenyl)-	149	C9H11NO	59
5.	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	46
6.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	43
7.	Phenol, 4-(2-methylpropyl)-	150	C10H14O	38
8.	Phenol, 4-butyl-	150	C10H14O	38
9.	BENZENE, 1-ETHOXY-4-ETHYL-	150	C10H14O	35
10.	Phenol, 2-methyl-4-(1,1,3,3-tetramethylb	220	C15H24O	35
11.	2-METHYL-3-INDAZOLONE-N-D1	148	C8H7DN2O	27
12.	1-(6-METHYL-2-PYRIDYL)PROPAN-2-ONE	149	C9H11NO	27
13.	2,3,4,5,6-Pentamethylpyridine	149	C10H15N	27
14.	1,2-Benzenedicarboxylic acid, diethyl es	222	C12H14O4	27
15.	5-methyl-7-amino-S-triazolo(1,5-A)pyrimi	149	C6H7N5	27
16.	Phenol, 2-(1,1-dimethylethyl)-6-methyl-	164	C11H16O	27
17.	TRIMETHYLSILYL-BUTADIYNE	122	C7H10Si	25
18.	Phenol, 4-(2-phenylethyl)-	198	C14H14O	22
19.	Phenol, 4-propyl-	136	C9H12O	22
20.	Benzenepropanoic acid, .alpha.,4-dihydro	196	C10H12O4	22

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	64	025154-52-3	129725	70	41	1	97	19	37	2	38	9633
2.	*64	000103-89-9	123491	36	48	0	99	25	37	18	43	8242
3.	64	000000-00-0	129728	70	41	1	97	19	37	2	38	9633
4.	*59	000537-92-8	123489	52	35	1	99	25	33	16	41	8232
5.	*46	000120-66-1	123488	34	50	0	79	41	20	18	43	8431
6.	*43	000103-89-9	12284	45	43	0	81	41	18	11	38	8899
7.	*38	004167-74-2	12724	55	32	0	58	55	14	0	49	6336
8.	*38	001638-22-8	12720	58	24	0	58	57	14	0	56	6175
9.	*35	000000-00-0	12763	44	43	0	59	53	11	15	43	6424
10.	*35	002219-84-3	43899	52	52	2	85	53	11	19	40	7298
11.	*27	054120-67-1	11923	41	47	2	99	60	8	14	40	7118
12.	27	065702-08-1	12327	44	40	1	79	59	8	0	39	6668
13.	*27	003748-83-2	12343	33	59	3	83	57	8	0	39	6889
14.	27	000084-66-2	44597	44	57	1	73	56	8	16	38	7052
15.	*27	033376-96-4	12206	37	32	3	99	58	8	0	41	6921
16.	27	002219-82-1	18585	57	37	2	89	58	8	0	39	7608
17.	*25	000000-00-0	4378	51	28	0	59	62	7	23	44	5979
18.	22	006335-83-7	34097	56	24	0	65	62	5	2	41	5977
19.	*22	000645-56-7	121890	45	31	0	65	62	5	11	40	5978
20.	22	051095-47-7	32695	47	58	0	70	62	5	0	39	5979

Nonylphenol Isomer [10]



Scan 1630 (29.915 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.15	232	69.00	95	95.00	199	119.15	125
50.70	54	71.15	59	97.15	91	120.00	112
51.80	35	71.50	40	99.30	25	121.15	1443
53.05	93	71.75	37	100.80	19	122.15	167
54.20	32	77.05	253	103.05	74	123.15	116
57.05	131	79.05	134	107.05	1806	125.20	59
58.45	35	81.05	75	108.05	136	131.05	76
59.20	29	82.05	68	109.05	57	133.20	101
64.15	53	85.20	26	110.80	64	134.05	200
65.00	176	91.15	282	112.00	43	135.05	2101
67.00	71	94.25	57	115.15	73	136.05	329

Scan 1630 (29.915 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.20	32						
139.40	19						
143.15	56						
147.15	49						
149.15	241						
150.25	46						
163.20	1035						
164.15	148						
191.25	33						
199.65	28						
220.25	75						

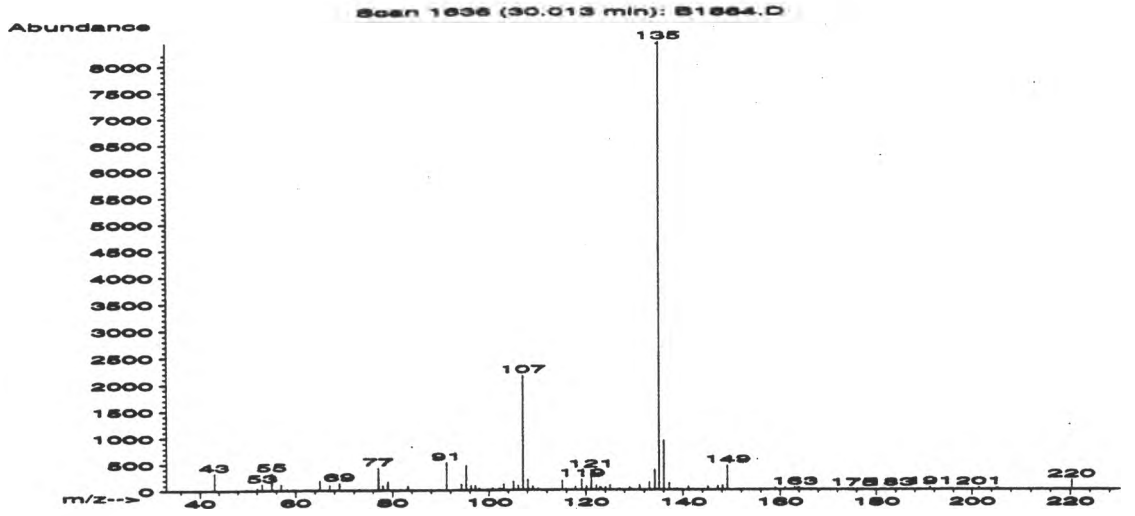
Scan 1630 (29.915 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	NONYLPHENOL ISOMER	220	C15H24O	59
2.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	53
3.	2-NONYLPHENOL	220	C15H24O	53
4.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	53
5.	Phenol, nonyl-	220	C15H24O	52
6.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	50
7.	Hexestrol	270	C18H22O2	50
8.	NONYLPHENOL ISOMER	220	C15H24O	35
9.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	35
10.	NONYLPHENOL ISOMER	220	C15H24O	30
11.	Benzene, (1-ethoxyethyl)-	150	C10H14O	27
12.	Adenine	135	C5H5N5	22
13.	1-(6-METHYL-2-PYRIDYL)PROPAN-2-ONE	149	C9H11NO	22
14.	Phenol, 4-propyl-	136	C9H12O	22
15.	Phenol, 4-propyl-	136	C9H12O	22
16.	Benzothiazole	135	C7H5NS	22
17.	(Z)-2,3-DIMETHYL-4-(2',6',6'-TRIMETHYL-1	220	C15H24O	22
18.	9-METHL-10-AZATRICYCLO[5.2.2.0(1,5)]UNDE	163	C11H17N	16
19.	Benzenepropanoic acid, .alpha.,4-dihydro	196	C10H12O4	14
20.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	59	000000-00-0	43895	69	43	0	93	23	33	0	39	8460
2.	53	000088-18-6	123666	44	49	2	86	29	28	16	38	8403
3.	*53	000136-83-4	44071	59	62	2	99	27	28	16	38	9311
4.	53	000088-18-6	12725	49	40	1	85	30	28	5	38	8326
5.	*52	025154-52-3	43894	52	75	2	84	35	27	0	46	9087
6.	50	000585-34-2	123672	44	46	2	82	32	25	17	39	7977
7.	50	000084-16-2	132208	60	56	1	99	32	25	0	39	8381
8.	35	000000-00-0	129727	58	47	2	173	55	11	0	43	8512
9.	35	000140-66-9	128869	44	61	1	99	51	11	14	41	7118
10.	*30	000000-00-0	129726	57	73	0	60	60	9	3	46	8959
11.	*27	003299-05-6	12765	42	47	1	71	56	8	13	40	8462
12.	*22	000073-24-5	121688	34	50	2	99	63	5	0	39	6509
13.	*22	065702-08-1	12327	36	48	0	77	64	5	0	41	5486
14.	*22	000645-56-7	121890	39	41	1	77	65	5	1	40	5506
15.	*22	000645-56-7	7897	33	55	2	85	63	5	0	41	5720
16.	*22	000095-16-9	121696	35	51	3	90	61	5	0	41	6390
17.	*22	059744-14-8	43966	34	76	2	97	63	5	10	39	6385
18.	*16	000000-00-0	18132	31	32	0	46	59	3	10	37	7299
19.	14	051095-47-7	127956	55	37	1	85	68	2	7	38	5435
20.	*12	015816-45-2	7331	44	36	1	99	64	2	1	36	6392

Nonylphenol Isomer [11]



Scan 1636 (30.013 min): B1664.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	333	77.05	428	102.05	25	117.90	61
49.80	20	78.05	87	102.45	31	119.15	207
52.05	41	79.05	163	103.05	118	120.15	76
53.05	124	83.20	79	105.05	168	121.15	378
55.05	330	91.15	530	106.05	85	122.15	84
56.95	117	94.15	116	107.05	2164	122.90	45
58.20	32	95.15	468	108.05	203	123.15	50
65.00	182	96.15	81	109.05	74	124.00	56
67.00	100	97.15	78	110.20	29	125.05	91
69.00	139	98.00	34	115.15	179	126.95	33
73.05	18	100.80	37	115.90	26	129.05	47

Scan 1636 (30.013 min): B1664.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
131.05	90	149.15	466	204.95	34		
133.05	154	159.05	37	205.20	33		
134.20	383	161.05	36	220.25	183		
135.05	8437	163.05	45				
136.05	941	163.70	34				
137.20	127	163.95	36				
138.75	28	164.65	19				
141.15	63	175.25	22				
145.15	60	183.05	23				
147.15	65	191.15	50				
148.15	86	201.40	42				

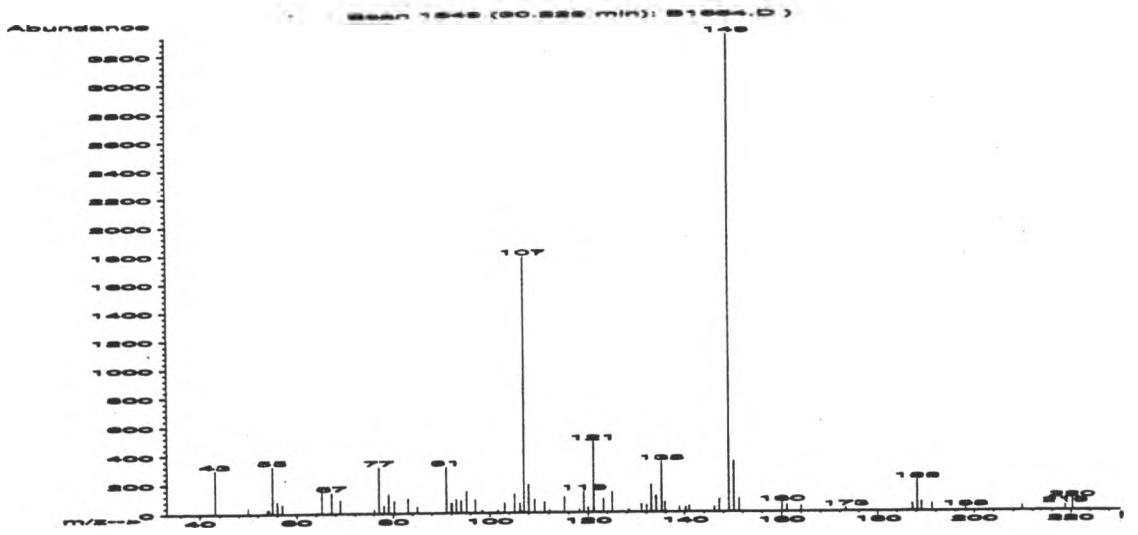
Scan 1636 (30.013 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	72
2.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	72
3.	NONYLPHENOL ISOMER	220	C15H24O	72
4.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	64
5.	OCTYL PHENOL ISOMER	206	C14H22O	64
6.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	50
7.	Phenol, 4-(1,1,3,3-tetramethylbutyl)-	206	C14H22O	50
8.	Phenol, 4-(2,2,3,3-tetramethylbutyl)-	206	C14H22O	50
9.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	50
10.	6-METHYL-TRIAZOLO[4,3-B]-1,2,4-TRIAZINE	135	C5H5N5	50
11.	Phenol, 4-nonyl-	220	C15H24O	46
12.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	43
13.	NONYLPHENOL ISOMER	220	C15H24O	42
14.	Silane, trichloro(2-tricyclo[3.3.1.1(3,7	296	C12H19Cl3Si	42
15.	Benzaldehyde, 4-methyl-, oxime	135	C8H9NO	42
16.	Adenine	135	C5H5N5	42
17.	Bicyclo[2.2.1]hept-2-en-7-ol, 7-(4-metho	216	C14H16O2	42
18.	ADAMANTANE, 1-BROMO-	214	C10H15Br	42
19.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	39
20.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	39

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	000585-34-2	123671	45	34	1	88	14	42	1	38	9932
2.	72	000089-83-8	123683	44	47	2	80	12	42	13	38	9939
3.	72	000000-00-0	129727	62	35	2	99	14	42	8	39	9840
4.	64	000140-66-9	128869	58	46	2	88	18	37	0	43	9915
5.	64	000000-00-0	37565	43	40	1	81	20	37	0	39	9935
6.	50	000140-66-9	128870	49	40	2	99	16	25	1	36	9903
7.	50	000140-66-9	37577	39	51	1	99	18	25	0	33	9849
8.	50	054932-78-4	37578	39	51	1	99	18	25	0	33	9854
9.	50	000098-54-4	123676	44	41	1	76	18	25	7	35	9919
10.	*50	061139-69-3	7509	28	81	0	98	20	25	0	33	9942
11.	*46	000104-40-5	129723	45	73	3	54	43	20	0	44	9471
12.	43	000098-54-4	123674	39	40	0	59	45	18	7	43	9904
13.	42	000000-00-0	43895	59	52	2	80	27	17	0	31	9796
14.	42	037843-11-1	72266	43	72	2	68	29	17	0	37	9757
15.	*42	003235-02-7	7571	31	58	2	92	27	17	0	33	9740
16.	*42	000073-24-5	121689	29	62	2	99	29	17	0	33	9694
17.	42	013143-81-2	42087	51	44	0	72	27	17	6	31	9706
18.	42	000000-00-0	129302	48	49	2	78	30	17	0	35	9782
19.	39	000585-34-2	123673	39	52	1	84	18	15	0	28	9948
20.	39	000585-34-2	12726	49	43	1	68	20	15	0	27	9917

Nonylphenol Isomer [12]



Scan 1649 (30.228 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.15	297	77.05	316	95.15	145	112.25	20
49.95	36	78.05	53	97.00	89	115.15	106
54.05	26	79.05	131	98.40	19	118.25	19
54.30	24	80.20	82	101.70	18	119.15	140
55.05	322	83.05	98	103.05	70	120.00	32
56.05	83	84.95	43	105.05	128	121.15	484
57.05	63	91.00	313	106.20	65	123.15	92
65.15	158	91.90	66	107.05	1785	124.95	139
67.15	142	92.15	64	108.05	189	128.45	18
69.00	91	93.00	93	109.20	92	130.95	53
76.05	26	94.00	86	111.20	71	132.05	46

Scan 1649 (30.228 min): B1664.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.05	187	151.20	90	218.75	35		
134.05	112	160.05	57	220.25	77		
135.20	342	161.05	47				
135.95	68	164.00	37				
138.90	34	173.25	22				
140.25	30	187.20	50				
141.00	41	188.20	210				
146.15	32	189.05	65				
147.15	86	191.15	50				
149.15	3327	198.15	18				
150.15	345	209.80	33				

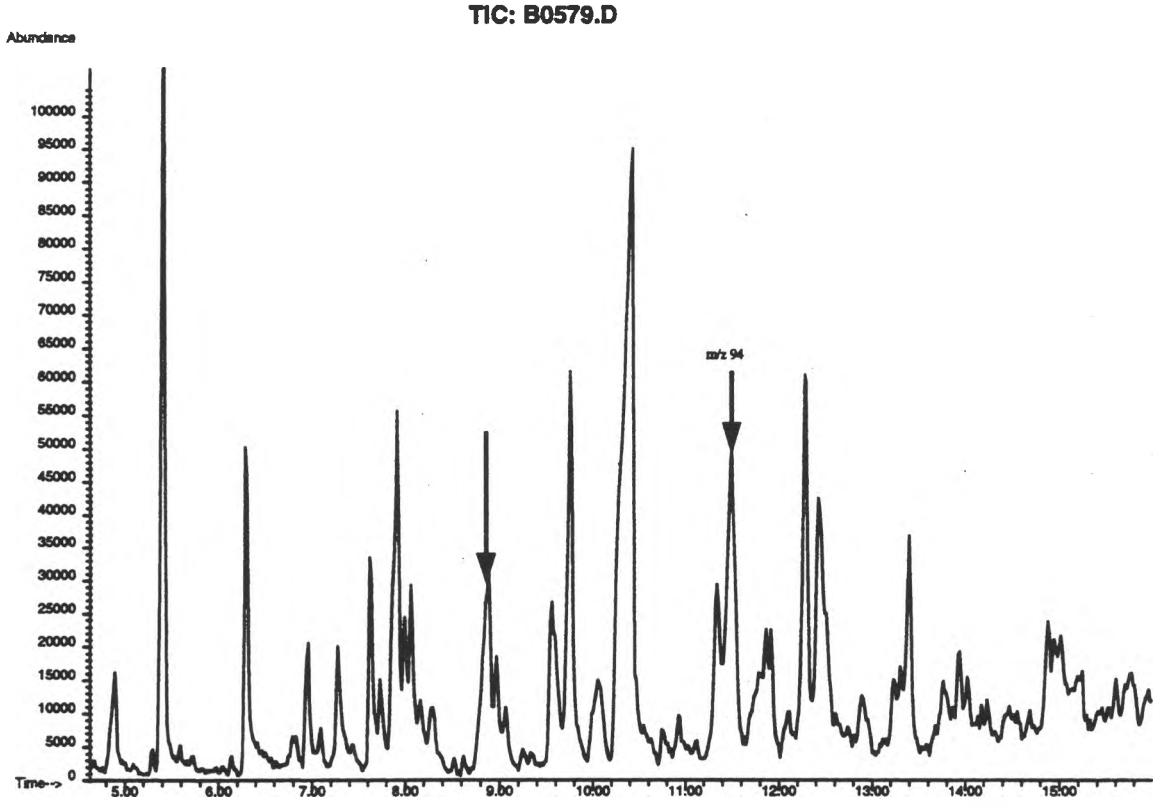
Scan 1649 (30.228 min): B1664.D

PBM Search of library D:\DATABASE\WILEY138.L

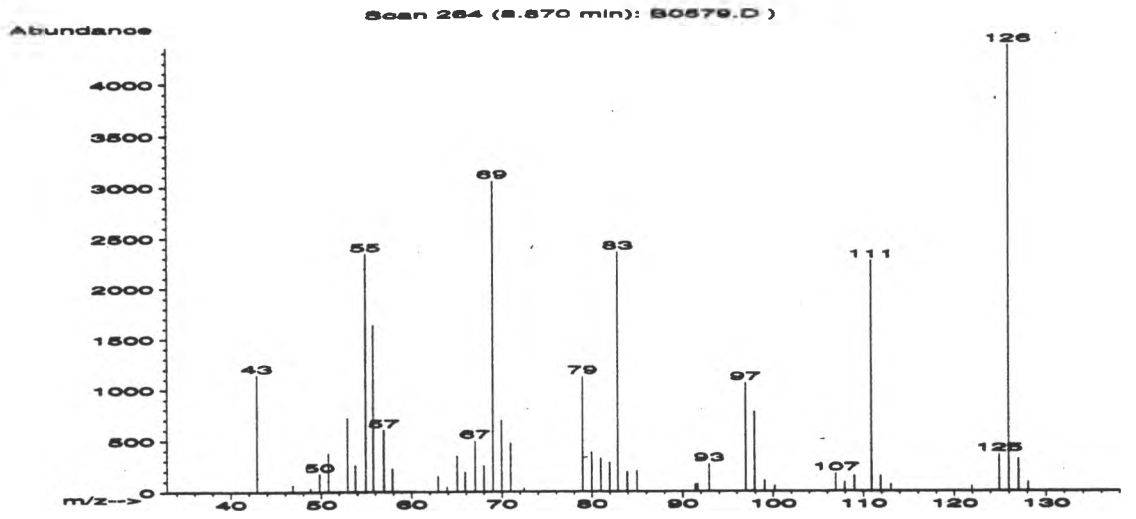
	Name	MolWt	Formula	Qual
1.	1-(6-METHYL-2-PYRIDYL)PROPAN-2-ONE	149	C9H11NO	59
2.	Phenol, nonyl-	220	C15H24O	53
3.	NONYLPHENOL ISOMER	220	C15H24O	53
4.	Phenol, 2-methyl-4-(1,1,3,3-tetramethylb	220	C15H24O	52
5.	Acetamide, N-(4-methylphenyl)-	149	C9H11NO	47
6.	1,3-CYCLOHEXADIENE, 1,3,5,5,6,6-HEXAMETH	164	C12H20	40
7.	CYCLOHEXYL PENTYL PHTHALATE	318	C19H26O4	38
8.	1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	37
9.	Benzene, 1-butyl-4-methoxy-	164	C11H16O	37
10.	1H-s-Triazolo[1,5-a]pyridin-4-ium, 2-hyd	149	C7H7N3O	37
11.	Tricyclo[4.3.1.1(3,8)]undecane-1-carboxy	208	C13H20O2	37
12.	1,2-Benzenedicarboxylic acid, dipropyl e	250	C14H18O4	32
13.	Tricyclo[4.3.1.1(3,8)]undecane, 1-bromo-	228	C11H17Br	22
14.	BENZENE, 1-ETHOXY-4-ETHYL-	150	C10H14O	22
15.	2,5-Cyclohexadien-1-one, 4-ethyl-3,4-dim	150	C10H14O	16
16.	Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-tri	150	C10H14O	11
17.	Phenol, 4-butyl-	150	C10H14O	10
18.	3-BUTYL-5-METHYL-1,2,3,8A-TETRAHYDROINDO	191	C13H21N	10
19.	Pyridine, 2,3-dimethyl-	107	C7H9N	10
20.	Benzenepropanoic acid, .alpha.,4-dihydro	196	C10H12O4	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	065702-08-1	12327	37	46	2	73	24	33	18	40	5520
2.	*53	025154-52-3	129725	60	52	0	53	36	28	0	56	9757
3.	*53	000000-00-0	129728	60	52	0	53	36	28	0	56	9757
4.	*52	002219-84-3	129729	51	56	1	78	34	27	0	46	8933
5.	*47	000103-89-9	12284	39	45	0	75	36	20	18	38	8942
6.	40	000000-00-0	18723	46	52	2	69	33	16	0	35	9627
7.	38	000000-00-0	79548	46	62	2	73	46	14	10	41	8716
8.	37	042541-33-3	37086	38	76	3	79	42	13	0	33	8185
9.	37	018272-84-9	18596	42	51	3	81	42	13	4	33	8971
10.	*37	013980-64-8	12217	30	60	2	79	42	13	4	37	8959
11.	37	031083-60-0	38597	43	66	2	79	43	13	0	34	9114
12.	32	000131-16-8	56409	44	58	1	71	46	9	0	35	8706
13.	22	021898-96-4	47500	44	62	1	64	62	5	11	38	9307
14.	*22	000000-00-0	12763	40	33	0	46	63	5	13	40	4860
15.	*16	017429-35-5	12775	43	40	2	48	59	3	9	33	4926
16.	*11	018309-32-5	12853	47	47	0	13	78	2	0	44	4350
17.	*10	001638-22-8	12720	28	38	0	39	69	1	0	33	4773
18.	10	000000-00-0	30455	46	39	0	51	75	1	19	41	4696
19.	*10	000583-61-9	118611	33	44	0	36	76	1	0	41	4632
20.	9	051095-47-7	32695	38	54	0	53	75	1	10	35	4638

BKME P&G Check



Peak 91



Scan 264 (8.870 min): B0579.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1143	62.90	147	79.95	380	99.05	100
46.80	70	63.90	52	80.95	319	100.20	50
48.80	39	65.00	347	81.95	280	106.95	166
49.80	171	65.90	190	82.90	2349	107.90	86
50.80	372	67.00	492	83.90	191	109.00	145
52.95	718	68.00	249	85.00	200	110.90	2260
53.80	255	69.00	3043	91.40	68	111.90	145
54.95	2338	69.95	694	91.65	70	113.00	67
55.80	1633	70.95	473	92.90	262	121.95	48
56.95	600	72.45	38	96.95	1058	124.95	352
57.90	220	78.95	1124	97.95	771	125.95	4350

Scan 264 (8.870 min): B0579.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.05	311						
128.05	85						

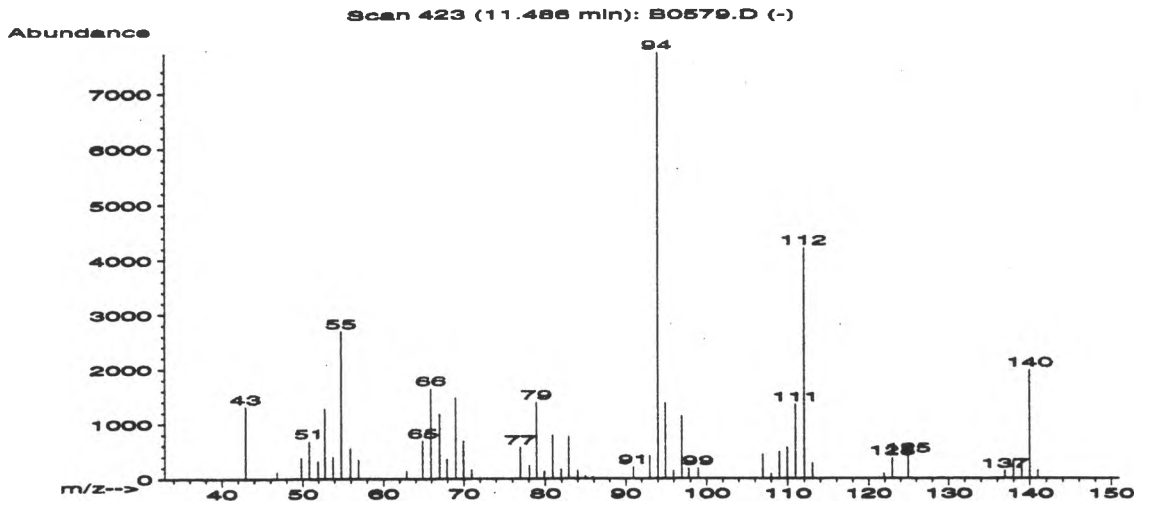
Scan 264 (8.870 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3,5-DIMETHYL-CYCLOPENTANE-1,2-DIONE	126	C7H10O2	64
2.	3,5-DIMETHYL-CYCLOPENTANE-1,2-DIONE	126	C7H10O2	62
3.	Benzene, 1-fluoro-4-methoxy-	126	C7H7FO	52
4.	1H-Pyrazole, 3-ethyl-4,5-dihydro-1,4-dim	126	C7H14N2	50
5.	Benzene, 1-fluoro-2-methoxy-	126	C7H7FO	46
6.	.DELTA.2-Tetrazaboroline, 5-ethyl-1,4-di	126	C4H11BN4	38
7.	4H-Pyran-4-one, 3-hydroxy-2-methyl-	126	C6H6O3	38
8.	Methyl cinnamate	126	C6H6O3	35
9.	4H-Pyran-4-one, 5-hydroxy-2-methyl-	126	C6H6O3	30
10.	4(1H)-Pyrimidinone, 2,6-diamino-	126	C4H6N4O	27
11.	Furan, 2,5-dihydro-2,5-dimethyl-	98	C6H10O	11
12.	3-Penten-2-one, 4-methyl-	98	C6H10O	11
13.	Cyclohexane, methyl-	98	C7H14	11
14.	Furan, 2,5-dihydro-3,4-dimethyl-	98	C6H10O	11
15.	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	10
16.	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	10
17.	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	10
18.	2-Pentene, 2,4-dimethyl-	98	C7H14	10
19.	2-Pentene, 2,4-dimethyl-	98	C7H14	10
20.	2-Pentene, 2,4-dimethyl-	98	C7H14	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	021834-98-0	120558	54	46	1	81	24	37	0	49	9636
2.	*62	021834-98-0	5204	65	44	1	75	28	36	0	58	9322
3.	*52	000459-60-9	120549	56	38	0	75	31	27	0	49	9162
4.	*50	075011-91-5	5272	36	71	3	159	32	25	0	41	7988
5.	*46	000321-28-8	120548	45	45	0	68	43	20	0	44	8576
6.	*38	020534-01-4	5088	47	47	2	67	46	14	12	41	7843
7.	*38	000118-71-8	120513	44	64	2	82	50	14	0	40	8014
8.	*35	061892-88-4	5130	36	64	3	99	53	11	0	41	7756
9.	*30	000644-46-2	5133	46	45	3	93	57	9	7	47	7516
10.	*27	000056-06-4	5075	46	59	1	76	57	8	0	40	7789
11.	*11	059242-27-2	879	45	42	0	38	72	2	0	44	4929
12.	*11	000141-79-7	117729	35	18	0	53	79	2	4	43	4147
13.	*11	000108-87-2	117819	46	50	0	53	75	2	0	44	4704
14.	*11	053720-72-2	880	33	41	0	47	77	2	18	43	3785
15.	*10	000762-63-0	927	35	55	0	53	77	1	0	41	4388
16.	*10	000690-08-4	117808	35	47	0	53	77	1	0	41	4332
17.	*10	000690-08-4	928	35	55	0	53	77	1	0	41	4346
18.	*10	000625-65-0	117804	35	48	0	53	77	1	0	41	4440
19.	*10	000625-65-0	117803	35	48	0	53	77	1	0	41	4401
20.	*10	000625-65-0	924	35	55	0	53	77	1	0	41	4338

Peak 92



Scan 423 (11.486 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1313	64.90	686	80.90	789	96.95	1139
46.80	115	65.90	1647	81.95	170	97.80	182
49.80	376	67.00	1177	82.90	767	98.95	186
50.80	685	67.90	357	84.00	146	106.95	436
51.95	312	69.00	1480	84.95	45	108.00	78
52.80	1276	69.95	691	85.90	32	109.00	481
53.80	398	70.95	157	90.95	208	109.95	559
54.80	2687	76.95	566	93.00	414	111.00	1351
55.95	548	78.05	236	94.00	7727	112.00	4211
56.95	342	78.95	1389	94.95	1375	113.00	282
62.85	136	79.90	128	95.95	139	121.90	80

Scan 423 (11.486 min): B0579.D

Modified:subtracted clipped

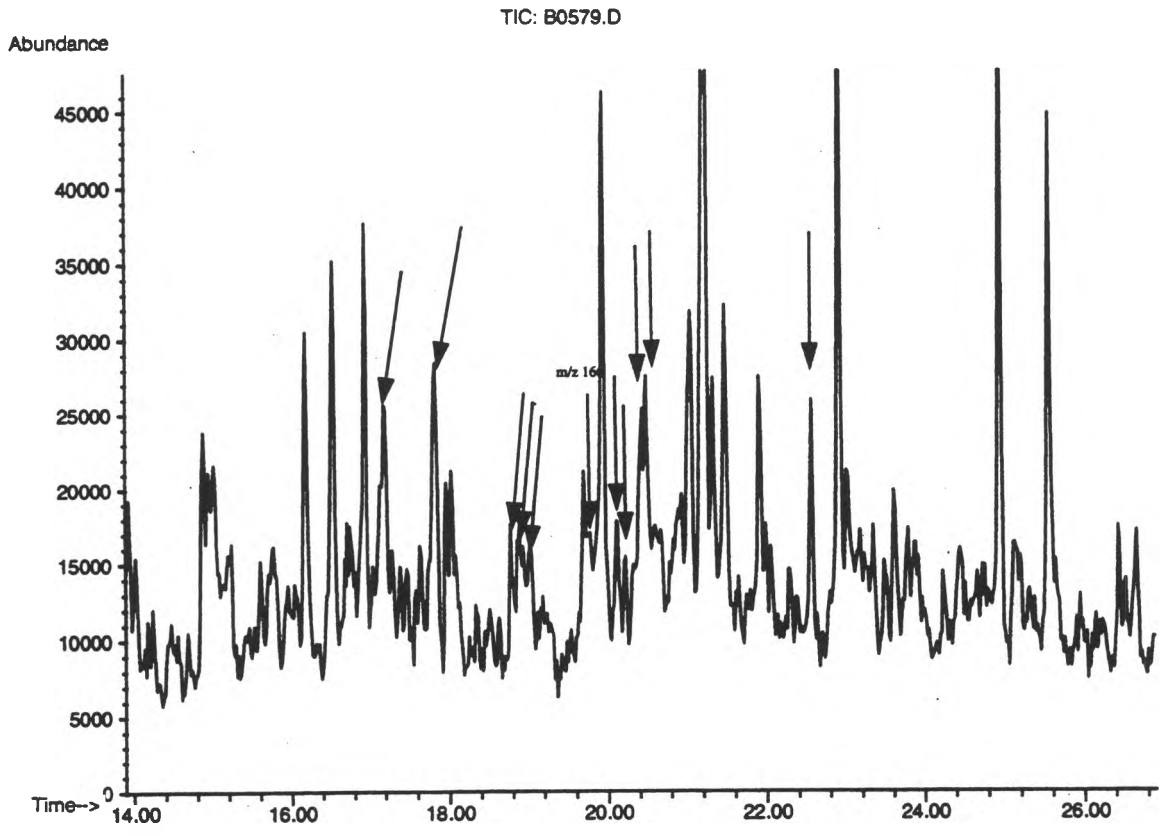
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.95	367						
124.95	416						
136.90	132						
137.95	304						
139.00	300						
140.00	1980						
141.00	147						

Scan 423 (11.486 min): B0579.D

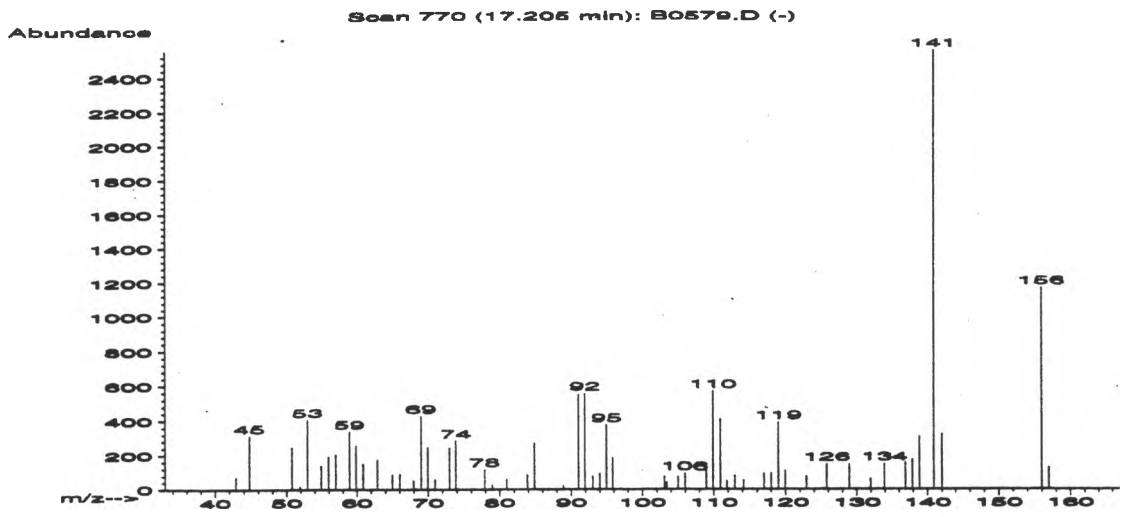
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol	94	C6H6O	38
2.	3-Furancarboxylic acid	112	C5H4O3	35
3.	3-Pyridinol, 2-nitro-	140	C5H4N2O3	32
4.	Bicyclo[2.2.1]heptan-7-ol	112	C7H12O	25
5.	2-Pyridinamine	94	C5H6N2	22
6.	2-Pyridinamine	94	C5H6N2	22
7.	Ethanol, 2-phenoxy-	138	C8H10O2	22
8.	8-Azabicyclo[3.2.1]oct-6-en-3-one, 8-met	137	C8H11NO	14
9.	Pyrimidine, 5-methyl-	94	C5H6N2	14
10.	Ethanol, 2-phenoxy-	138	C8H10O2	12
11.	2-Pyridinamine	94	C5H6N2	12
12.	4-Pyridinamine	94	C5H6N2	12
13.	4-Pyridinamine	94	C5H6N2	12
14.	8-Azabicyclo[3.2.1]oct-6-en-3-ol, 8-meth	139	C8H13NO	12
15.	Benzene, 1-ethoxy-4-fluoro-	140	C8H9FO	10
16.	2(1H)-Pyridinone, 1,5-dimethyl-	123	C7H9NO	10
17.	1-Carbethoxyethylidenecyclopropane	140	C8H12O2	10
18.	3-Cyclohexene-1-acetaldehyde, .alpha.,4-	152	C10H16O	10
19.	8-Azabicyclo[3.2.1]oct-6-en-3-ol, 8-meth	139	C8H13NO	10
20.	4-ETHYL-2-METHYL-1,3-CYCLOPENTADIONE	140	C8H12O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	000108-95-2	117519	28	60	2	98	37	14	3	30	8397
2.	*35	000488-93-7	2425	34	85	3	93	54	11	0	41	3812
3.	*32	015128-82-2	9020	34	52	1	48	46	9	0	30	8468
4.	*25	002566-48-5	2611	53	51	2	89	45	7	0	28	9129
5.	*22	000504-29-0	117510	33	49	1	80	64	5	0	39	8415
6.	*22	000504-29-0	117509	33	57	2	67	64	5	0	39	8421
7.	*22	000122-99-6	8518	33	50	1	80	62	5	11	40	8237
8.	*14	004438-38-4	8313	43	38	0	89	66	2	18	40	8300
9.	*14	002036-41-1	468	40	35	0	87	66	2	0	39	8378
10.	*12	000122-99-6	122231	28	33	1	76	63	2	12	34	7715
11.	*12	000504-29-0	471	33	55	1	99	64	2	0	30	8395
12.	*12	000504-24-5	117514	34	50	2	92	64	2	0	35	8379
13.	*12	000504-24-5	473	29	51	2	99	64	2	0	33	8383
14.	*12	020513-09-1	8951	28	53	3	93	63	2	2	35	8323
15.	*10	000459-26-7	122435	43	41	1	53	75	1	0	40	4991
16.	*10	006456-93-5	4562	39	38	1	69	66	1	15	36	8272
17.	10	055281-62-4	9191	44	23	0	42	73	1	16	41	5009
18.	10	029548-14-9	13658	43	48	2	97	66	1	0	37	8296
19.	*10	054725-49-4	122380	29	60	2	77	62	1	0	29	8358
20.	10	000000-00-0	9206	46	57	2	53	70	1	0	37	5994


TIC: B0579.D
Abundance
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
Time-->
14.00
16.00
18.00
20.00
22.00
24.00
26.00

Peak 93



Scan 770 (17.205 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	74	62.90	173	81.00	60	103.05	76
44.80	317	65.00	89	83.90	87	103.45	42
50.75	246	66.00	91	84.90	271	105.00	75
51.85	18	67.95	53	88.90	23	105.95	96
52.95	408	69.00	429	91.00	551	108.95	126
54.90	140	69.95	247	91.90	559	109.90	570
55.95	193	70.95	60	93.00	78	110.90	411
56.95	205	72.95	245	94.00	97	111.80	49
58.90	338	73.80	286	94.95	376	112.90	83
59.85	256	77.85	119	95.80	182	114.15	53
60.85	151	78.95	27	96.95	7	117.00	94

Scan 770 (17.205 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
118.00	97	140.90	2557				
119.00	392	142.00	321				
119.95	109	155.95	1169				
122.95	78	156.95	129				
125.80	149						
128.95	147						
131.95	63						
133.90	150						
136.90	159						
137.90	173						
138.90	307						

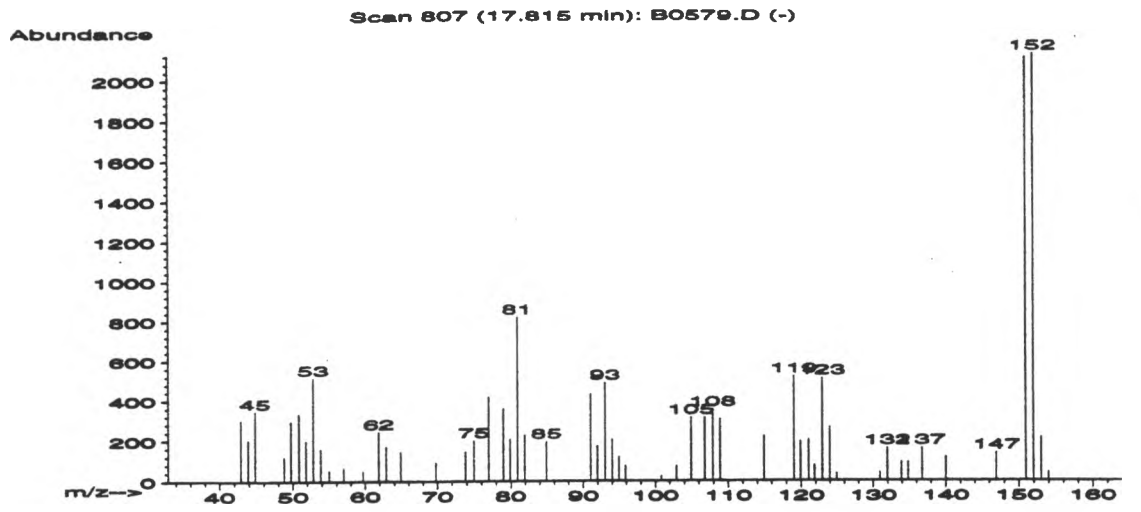
Scan 770 (17.205 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1,2-Difluoro-3,4,5-trimethylbenzene	156	C9H10F2	74
2.	5-ETHYL-2-THIOPHENECARBOXYLIC ACID	156	C7H8O2S	52
3.	Naphthalene, 1-ethyl-	156	C12H12	49
4.	Naphthalene, 1-ethyl-	156	C12H12	47
5.	Naphthalene, 1-ethyl-	156	C12H12	47
6.	Naphthalene, 2-ethyl-	156	C12H12	47
7.	Naphthalene, 2-ethyl-	156	C12H12	47
8.	Naphthalene, 1-ethyl-	156	C12H12	38
9.	Naphthalene, 1-ethyl-	156	C12H12	38
10.	Naphthalene, 1-ethyl-	156	C12H12	38
11.	Naphthalene, 2-ethyl-	156	C12H12	38
12.	Naphthalene, 2-ethyl-	156	C12H12	38
13.	2-Methylamino-4-isopropyl thiazole	156	C7H12N2S	28
14.	Naphthalene, 2-ethyl-	156	C12H12	28
15.	Thiazole, 2,4-diethyl-	141	C7H11NS	16
16.	Benzene, 1-fluoro-2-nitro-	141	C6H4FNO2	16
17.	2-Propanethione, 1-(2-pyrrolidinylidene)	141	C7H11NS	12
18.	Thiazole, 2,5-diethyl-	141	C7H11NS	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*74	085649-61-2	15328	32	17	0	70	0	44	0	33	9183
2.	*52	000000-00-0	15147	51	44	1	90	32	27	0	46	9419
3.	*49	001127-76-0	124564	33	53	0	85	38	23	10	43	9301
4.	*47	001127-76-0	124567	33	64	0	70	38	20	0	41	9312
5.	*47	001127-76-0	15645	33	65	0	75	38	20	0	41	9328
6.	*47	000939-27-5	124571	38	61	0	69	38	20	0	39	9322
7.	*47	000939-27-5	124570	33	63	0	72	38	20	0	41	9326
8.	*38	001127-76-0	124566	33	59	0	75	38	14	4	37	9314
9.	*38	001127-76-0	124565	33	59	0	75	38	14	4	37	9314
10.	*38	001127-76-0	124563	33	57	0	79	38	14	4	37	9313
11.	*38	000939-27-5	124569	33	59	0	77	38	14	4	37	9298
12.	*38	000939-27-5	124568	33	59	0	77	38	14	4	37	9298
13.	*28	080232-90-2	15194	31	59	1	83	40	8	0	26	9180
14.	*28	000939-27-5	15646	32	60	0	67	38	8	7	25	9292
15.	*16	032272-49-4	9643	31	54	2	99	59	3	7	34	8481
16.	*16	001493-27-2	9563	34	78	2	84	59	3	0	30	7615
17.	*12	054031-27-5	122550	28	82	2	89	59	2	0	26	8459
18.	*12	015729-76-7	9644	28	85	1	99	59	2	0	23	8375

Peak 94



Scan 807 (17.815 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	300	59.65	47	81.95	225	106.80	313
43.90	201	61.90	242	84.95	194	107.90	354
44.80	345	62.90	168	91.00	431	108.90	306
48.80	119	64.90	142	91.95	172	114.90	220
49.75	296	69.80	91	93.00	489	119.00	520
50.85	335	73.80	144	94.00	204	119.95	192
51.80	196	74.95	199	94.95	118	121.05	200
52.80	514	76.95	416	95.85	75	121.90	75
53.80	158	78.95	359	100.80	23	122.95	512
54.95	52	79.90	206	102.95	72	123.95	265
56.95	64	80.95	819	104.95	313	124.95	34

Scan 807 (17.815 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
130.95	39						
131.95	160						
133.90	91						
134.85	91						
136.75	160						
140.00	115						
146.95	136						
150.95	2107						
151.95	2125						
152.95	213						
153.95	42						

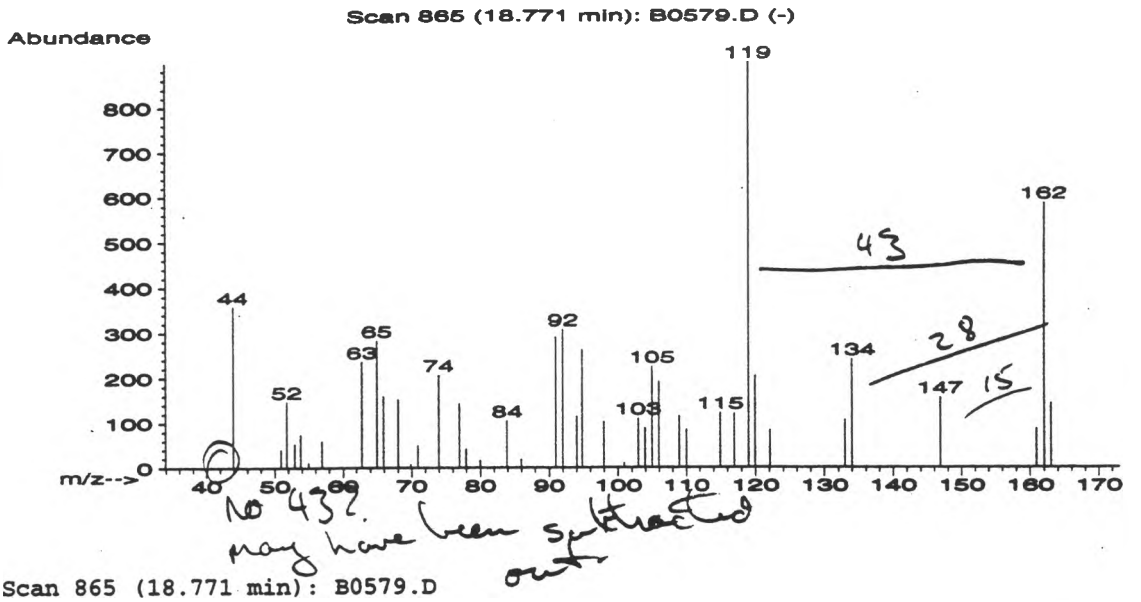
Scan 807 (17.815 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	74
2.	Benzaldehyde, 3-hydroxy-4-methoxy-	152	C8H8O3	74
3.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	72
4.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	72
5.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	68
6.	Benzaldehyde, 4-(methylthio)-	152	C8H8OS	53
7.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	52
8.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	52
9.	2-METHOXY-4,5,6-TRIMETHYLPYRIMIDINE	152	C8H12N2O	50
10.	Benzaldehyde, 3-(chloroacetoxy)-4-methox	228	C10H9ClO4	50
11.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	50
12.	3,5,6-Trimethylpyrazine-2-methanol	152	C8H12N2O	43
13.	1,4-Benzenediol, 2,3,5-trimethyl-	152	C9H12O2	35
14.	Benzaldehyde, 2-hydroxy-4-methoxy-	152	C8H8O3	35
15.	2,3,4,6-Tetramethyl-4-pyrone	152	C9H12O2	27
16.	N-PHENYL, N-DEUTERO-CARBAMIC ACID METHYL	151	C8H8DNO2	27
17.	Benzaldehyde, 3-methoxy-, oxime	151	C8H9NO2	27
18.	1,4-Benzodioxan-2-ol	152	C8H8O3	22
19.	N,N-DIMETHYL-N'-(2,4,6-TRI-DEUTEROPHENYL	148	C9H9D3N2	22
20.	Benzoic acid, 4-methoxy-	152	C8H8O3	18

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*74	000121-33-5	13356	66	46	2	99	20	44	0	58	9734
2.	*74	000621-59-0	123897	58	59	3	87	20	44	0	51	8596
3.	*72	000121-33-5	123898	50	76	3	99	20	42	0	46	9745
4.	*72	000121-33-5	123900	64	43	1	98	20	42	0	50	9745
5.	*68	000121-33-5	123901	59	49	2	99	24	40	0	51	9753
6.	*53	003446-89-7	13330	51	58	1	70	29	28	6	39	9773
7.	*52	000121-33-5	123899	44	43	0	91	33	27	0	44	9626
8.	*52	000121-33-5	123903	66	39	1	99	31	27	0	50	9740
9.	*50	065641-61-4	123916	33	50	1	96	33	25	15	40	9487
10.	50	066267-38-7	47410	60	66	1	97	31	25	0	39	9715
11.	*50	000121-33-5	123902	52	52	1	99	32	25	0	39	9750
12.	*43	075907-74-3	13394	36	60	1	74	43	18	21	40	8510
13.	*35	000700-13-0	13531	44	62	2	86	55	11	0	39	8371
14.	*35	000673-22-3	13357	45	53	3	154	52	11	0	39	9409
15.	*27	014901-87-2	13446	50	38	0	88	58	8	14	41	6006
16.	*27	056196-25-9	13088	48	57	1	99	58	8	0	39	7028
17.	*27	038489-80-4	13105	30	53	0	72	60	8	1	42	7537
18.	*22	005770-59-2	13372	47	59	2	92	64	5	0	40	6716
19.	*22	029366-16-3	11982	42	61	0	81	63	5	14	40	7766
20.	*18	000100-09-4	123887	48	25	0	73	68	3	0	46	6810

Peak 95



Scan 865 (18.771 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	357	69.85	8	94.80	262	119.00	898
50.90	41	70.90	50	97.95	103	119.95	204
51.75	147	73.95	206	100.90	11	122.05	83
52.95	54	76.95	143	102.90	110	132.95	106
53.80	74	77.95	42	103.90	88	134.00	240
54.95	12	79.95	17	104.95	224	146.85	156
56.90	60	83.90	105	105.95	191	160.90	87
62.75	235	85.95	19	109.00	115	162.00	584
64.95	282	90.95	290	110.00	85	163.00	143
65.90	159	92.00	306	114.95	122		
68.00	152	94.00	115	116.95	120		

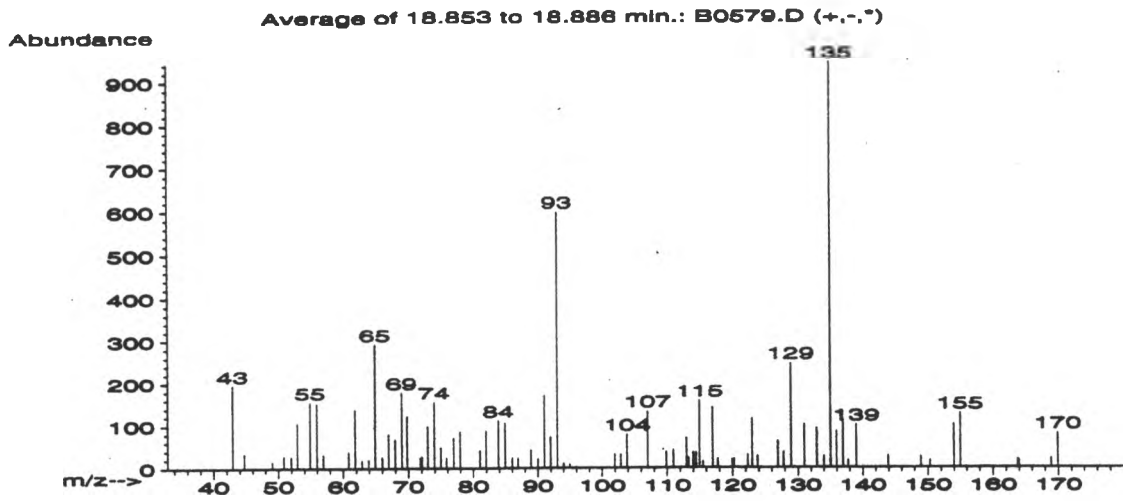
Scan 865 (18.771 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Bicyclo[3.2.2]nona-6,8-dien-3-one, 1,5-d	162	C11H14O	59
2.	2,4(1H,3H)-Quinazolinedione	162	C8H6N2O2	52
3.	1H-1,5-Benzodiazepine, 2,3,4,5-tetrahydr	162	C10H14N2	47
4.	Benzene, 1,4-dimethyl-2-(2-methylpropyl)	162	C12H18	43
5.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	38
6.	1,4-Cyclohexadiene, 3-ethenyl-1,2-dimeth	134	C10H14	35
7.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	35
8.	ORTHO-D2-BENZYLCYANIDE	117	C8H5D2N	30
9.	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	27
10.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14	27
11.	Benzene, 1-methyl-4-(1-methylethyl)-	134	C10H14	27
12.	HOMOCHROMANONE-5	162	C10H10O2	25
13.	2,4-DIHYDROXY-1,5-NAPHTHYRIDINE	162	C8H6N2O2	22
14.	.ALPHA.-D2-BENZYLCYANIDE	117	C8H5D2N	22
15.	Imidazo[1,2-a]pyrimidine	119	C6H5N3	22
16.	Ethanoadamantane	162	C12H18	22
17.	Benzene, 1-methyl-2-(1-ethylpropyl)-	162	C12H18	22
18.	Benzonitrile, 4-ethoxy-	147	C9H9NO	14
19.	2-Vinyladamantane	162	C12H18	14
20.	2,3-Quinoxalinedione, 1,4-dihydro-	162	C8H6N2O2	14

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	052114-13-3	17797	35	32	0	73	25	33	12	39	8473
2.	*52	000086-96-4	125073	36	65	0	78	32	27	4	43	8917
3.	*47	040358-34-7	17697	44	85	2	89	39	20	0	40	8998
4.	*43	055669-88-0	17845	52	41	0	92	44	18	6	41	8061
5.	*38	000099-87-6	7447	58	45	0	74	58	14	0	56	7605
6.	*35	062338-57-2	7463	46	53	0	77	53	11	5	40	7797
7.	*35	000099-87-6	121634	49	54	1	95	54	11	7	40	7741
8.	*30	053897-46-4	3681	44	70	0	99	60	9	14	47	7597
9.	*27	000933-98-2	121654	35	56	0	96	59	8	0	41	7517
10.	*27	000535-77-3	121630	36	56	0	99	59	8	0	41	7528
11.	*27	000099-87-6	121639	46	52	0	91	59	8	7	40	7491
12.	*25	006786-30-7	17656	33	65	0	45	64	7	22	43	6319
13.	*22	060058-16-4	17510	36	93	0	57	64	5	0	41	6086
14.	*22	000935-66-0	3680	33	79	1	85	62	5	0	39	7604
15.	*22	000274-95-3	3954	33	72	1	94	62	5	0	39	7596
16.	*22	015002-90-1	17920	33	45	0	52	63	5	0	41	7666
17.	*22	054410-74-1	17840	33	70	2	207	62	5	0	39	7240
18.	*14	025117-74-2	11644	35	72	0	67	66	2	0	41	7377
19.	*14	081372-28-3	17907	35	70	1	48	66	2	0	39	6958
20.	*14	015804-19-0	17508	35	50	0	45	69	2	0	41	5284

Peak 96



Average of 18.853 to 18.886 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	195	62.85	18	73.95	156	88.90	42
44.70	34	63.90	20	74.95	48	90.00	22
49.05	15	64.90	292	75.80	24	90.95	171
50.85	28	66.00	26	76.95	71	91.95	73
51.95	26	66.95	80	77.95	86	93.00	598
52.90	106	67.95	67	81.00	41	94.00	10
54.90	155	68.95	178	81.95	87	94.95	9
55.95	151	69.80	123	83.85	111	95.90	2
56.95	31	71.80	25	84.90	106	101.95	32
60.85	38	72.05	28	86.00	25	102.90	32
61.80	138	72.95	99	86.90	23	103.85	79

Average of 18.853 to 18.886 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.00	134	119.95	20	135.00	943	163.95	18
109.90	37	120.20	20	135.95	86	168.90	22
110.95	41	122.30	31	136.95	111	169.90	81
112.95	70	123.00	116	137.75	17		
113.25	24	123.80	29	139.00	101		
114.00	36	126.95	62	143.90	28		
114.40	36	127.80	36	148.95	26		
114.95	158	128.95	246	150.30	16		
115.50	15	130.95	102	153.95	102		
116.95	142	132.90	93	154.95	128		
117.75	22	134.00	27	163.75	20		

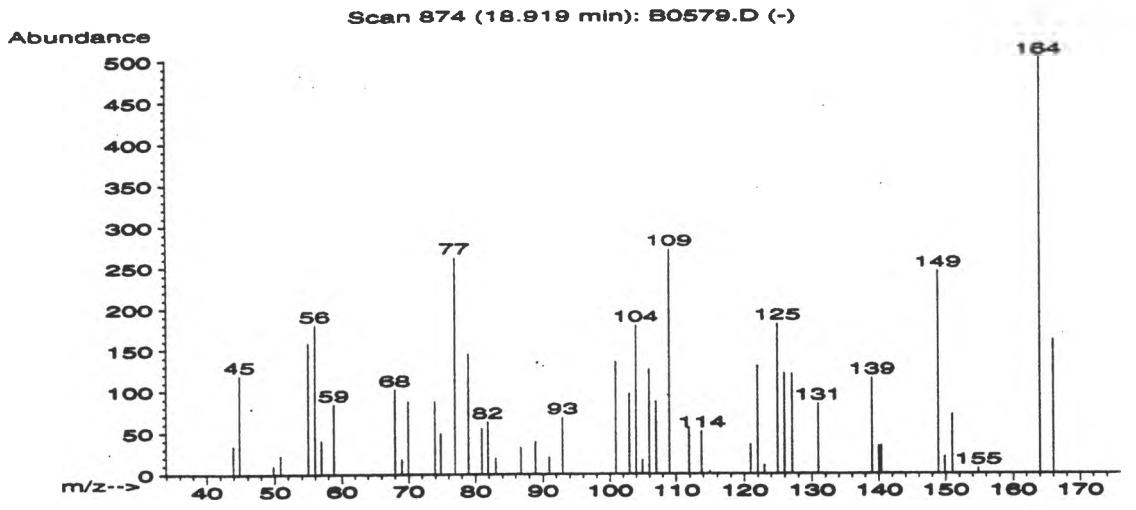
Average of 18.853 to 18.886 min.: B0579.D
Converted from RTE data file: >B0579:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	DIMETHYLPHOSPHINOTHIOIC AZIDE	135	C2H6N3PS	43
2.	Pyridine, 2-butyl-	135	C9H13N	37
3.	1,2-Benzisothiazole	135	C7H5NS	30
4.	1,2-Benzisothiazole	135	C7H5NS	30
5.	Benzoic acid, 4-(bromomethyl)-	214	C8H7BrO2	27
6.	Benzoyl chloride, 2-methoxy-	170	C8H7ClO2	27
7.	1,2-Benzisothiazole-3-carboxylic acid	179	C8H5NO2S	27
8.	Benzothiazole	135	C7H5NS	27
9.	Benzothiazole	135	C7H5NS	27
10.	Benzothiazole	135	C7H5NS	27
11.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	25
12.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	22
13.	1-Propanone, 1-(4-methoxyphenyl)-	164	C10H12O2	22
14.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	22
15.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	22
16.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	22
17.	3,4-DIETHYLPHENOL	150	C10H14O	12
18.	Adenine	135	C5H5N5	12
19.	.beta.-Phellandrene	136	C10H16	11
20.	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*43	027260-90-8	7490	42	60	3	99	42	18	0	39	9501
2.	*37	005058-19-5	121727	41	52	2	71	44	13	4	37	8105
3.	*30	000272-16-2	121700	44	45	2	95	58	9	0	44	8100
4.	*30	000272-16-2	7531	50	41	2	95	58	9	0	46	8103
5.	27	006232-88-8	40963	47	57	2	89	58	8	17	38	8084
6.	*27	021615-34-9	21131	38	33	0	78	59	8	5	40	8058
7.	27	040991-34-2	25013	43	55	2	95	58	8	0	39	8100
8.	*27	000095-16-9	121694	37	56	2	88	58	8	0	39	8107
9.	*27	000095-16-9	121696	33	55	2	99	58	8	0	39	8089
10.	*27	000095-16-9	121697	38	52	2	95	57	8	7	40	8099
11.	*25	000089-83-8	123679	53	35	0	90	61	7	10	43	8031
12.	*22	000499-75-2	123687	50	33	0	67	61	5	2	41	8031
13.	*22	000121-97-1	18420	46	28	0	70	61	5	19	40	8032
14.	*22	000089-83-8	123681	43	43	0	73	61	5	7	40	8031
15.	*22	000089-83-8	123680	52	34	0	93	61	5	18	43	8031
16.	22	000089-83-8	123685	50	37	1	93	61	5	8	41	8031
17.	12	000875-85-4	12892	44	56	2	99	65	2	0	35	8030
18.	*12	000073-24-5	121686	29	37	0	99	61	2	8	37	8031
19.	*11	000555-10-2	122038	37	49	0	63	78	2	14	43	5140
20.	*10	029548-02-5	8069	37	60	1	42	78	1	0	39	5121

Peak 97



Scan 874 (18.919 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.90	34	73.90	88	100.90	135	121.95	130
44.80	119	74.80	49	102.95	97	122.95	10
49.80	10	76.95	262	103.95	179	124.95	181
50.85	22	78.95	145	104.95	17	125.95	121
54.95	158	80.95	55	105.95	126	127.05	120
55.95	180	81.85	63	107.00	87	130.95	84
56.95	40	83.00	19	109.00	271	139.00	115
58.80	84	86.75	32	111.90	56	140.00	33
68.00	102	88.90	39	113.75	51	140.40	34
69.00	18	90.95	20	114.95	3	148.90	245
69.90	88	92.95	68	120.95	35	149.85	20

Scan 874 (18.919 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.95	71						
154.85	6						
164.00	501						
166.00	161						

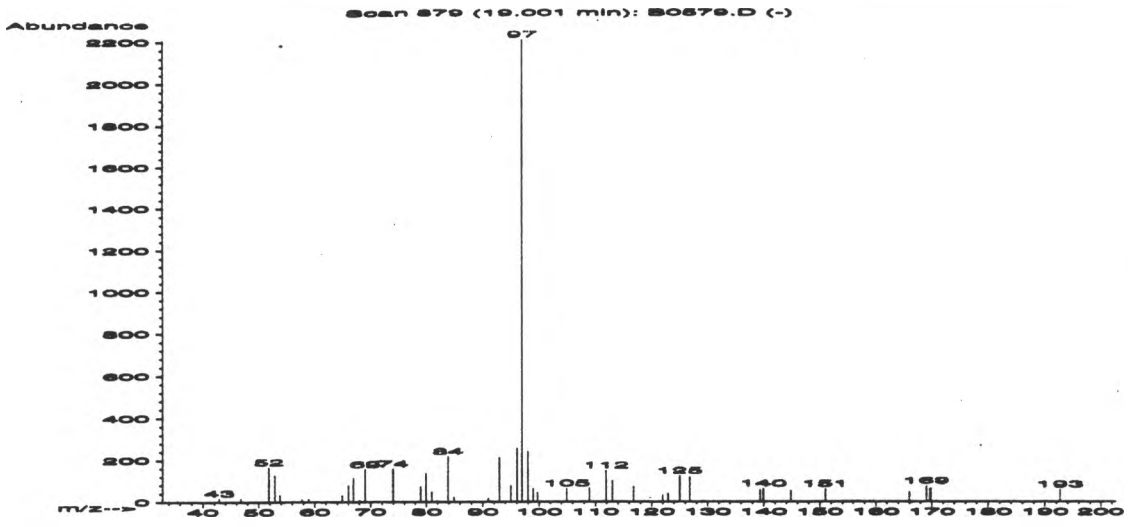
Scan 874 (18.919 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3,4-DIMETHYL-5,1'-BITRIAZOLE	164	C6H8N6	35
2.	7-Benzofuranol, 2,3-dihydro-2,2-dimethyl	164	C10H12O2	35
3.	Methanimidamide, N'-(4-hydroxyphenyl)-N,	164	C9H12N2O	27
4.	3-ALLYL-6-METHOXYPHENOL	164	C10H12O2	27
5.	cis-Jasmone	164	C11H16O	25
6.	Methanimidamide, N'-(3-hydroxyphenyl)-N,	164	C9H12N2O	22
7.	2-Cyclohexen-1-one, 6-[3-(acetyloxy)-1-m	224	C13H20O3	17
8.	1-ACETOXY-3-(4'-METHYL-2'OXO-CYCLOHEX-3'	224	C13H20O3	17
9.	6-METHYL-2,3-DIHYDRO-4-HYDROXY-2-METHYLB	164	C10H12O2	16
10.	Benzene, 4-ethenyl-1,2-dimethoxy-	164	C10H12O2	16
11.	Phenol, 2-methoxy-4-(1-propenyl)-	164	C10H12O2	16
12.	1-Benzothiepin, 2,3,4,5-tetrahydro-	164	C10H12S	12
13.	4H-Pyrido[1,2-a]pyrimidin-4-one, 6,7,8,9	164	C9H12N2O	12
14.	2-METHOXY-3,5-DIMETHYL-BENZALDEHYDE	164	C10H12O2	12
15.	5-ISOPROPYL-2-METHYL-1,4-BENZOQUINONE	164	C10H12O2	12
16.	Phenol, 2-methoxy-4-(1-propenyl)-	164	C10H12O2	10
17.	Phenol, 2-methoxy-4-(2-propenyl)-	164	C10H12O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*35	063523-90-0	18195	39	71	0	95	51	11	5	38	8079
2.	*35	001563-38-8	18472	43	78	1	72	55	11	0	40	8018
3.	*27	002350-51-8	18371	33	66	0	99	58	8	10	39	7898
4.	*27	000501-19-9	18510	56	57	0	83	58	8	5	38	7809
5.	*25	000488-10-8	125352	28	113	3	99	44	7	0	29	8741
6.	*22	025635-97-6	18370	35	71	0	95	62	5	10	39	7703
7.	17	077573-51-4	45802	35	45	0	99	51	3	0	25	8045
8.	17	062048-27-5	45807	35	45	0	99	51	3	0	25	8045
9.	*16	057330-85-5	18471	36	70	1	77	58	3	0	35	7847
10.	*16	006380-23-0	18442	38	63	1	95	57	3	0	33	7837
11.	*16	000097-54-1	125322	41	70	2	94	58	3	2	37	7834
12.	*12	004370-78-9	18523	29	86	1	95	56	2	0	29	7918
13.	*12	032092-29-8	18375	30	79	2	77	56	2	0	29	7944
14.	*12	016313-77-2	18411	31	47	0	93	65	2	0	33	7797
15.	*12	000000-00-0	18430	30	62	2	99	58	2	0	29	7814
16.	*10	000097-54-1	125324	31	78	1	77	65	1	0	29	7758
17.	*10	000097-53-0	125329	32	79	1	76	63	1	0	29	7867

Peak 98



Scan 879 (19.001 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	19	68.00	7	94.95	78	121.95	33
46.80	17	69.00	157	96.05	256	122.95	40
51.80	167	73.95	159	96.95	2207	125.00	125
52.90	128	78.95	74	97.95	241	126.80	117
53.80	34	79.95	138	98.95	65	139.40	57
55.85	4	80.95	48	99.70	46	139.95	63
57.70	13	81.95	6	104.95	65	144.80	53
58.90	15	83.90	218	108.95	67	150.95	62
64.90	32	84.90	24	111.90	151	165.95	46
66.00	79	90.95	18	113.00	100	169.00	76
66.95	115	92.95	213	116.75	73	169.65	61

Scan 879 (19.001 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
169.80	63						
192.65	59						

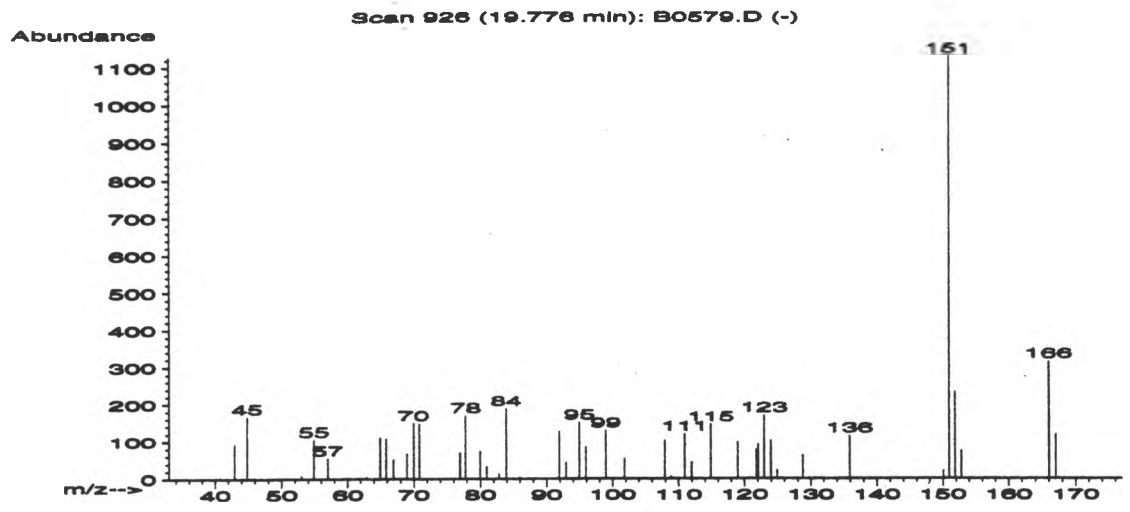
Scan 879 (19.001 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-METHOXY-2-ETHOXYETHYL-1-FURAN	170	C9H14O3	53
2.	SILANE, TRIMETHYL-2-PROPYNE-	112	C6H12Si	53
3.	2H-Pyrrol-2-one, 1,5-dihydro-1-methyl-	97	C5H7NO	53
4.	Cyclohexane, 1,1-dimethyl-	112	C8H16	42
5.	2-(N-BUTYL)-3,4,5,6-D4-PYRIDINE	135	C9H9D4N	40
6.	BICYCLO[3.3.1]NON-1-OL-3-ONE	154	C9H14O2	39
7.	(2R*,1'S*)-2-(1'-((Benzyloxy)methyl)prop	260	C16H20O3	38
8.	2-Butyne-1,4-diamine, N,N,N',N'-tetramet	140	C8H16N2	36
9.	METHYL 3-(2-THIENYL)PROPANOATE	170	C8H10O2S	33
10.	4-Hepten-3-one, 5-methyl-	126	C8H14O	33
11.	5-Nonen-4-one	140	C9H16O	33
12.	1-Pentyne, 3-ethyl-3-methoxy-	126	C8H14O	33
13.	Cyclohexane, 1-bromo-4-methyl-	176	C7H13Br	33
14.	3,4-DIMETHYL-ISOXAZOLE	97	C5H7NO	33
15.	Thiophene, 2-(2-ethylbutyl)-	168	C10H16S	28
16.	1,2-Ethanediol, 1,2-di-2-furanyl-	194	C10H10O4	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	000000-00-0	21280	37	61	2	77	30	28	0	39	7971
2.	*53	000000-00-0	2532	41	38	0	68	30	28	0	39	9849
3.	*53	013950-21-5	677	34	58	2	130	28	28	0	39	9855
4.	*42	000590-66-9	2721	29	36	1	77	26	17	6	35	9904
5.	*40	000000-00-0	7595	24	43	1	99	35	16	5	32	9870
6.	39	020498-02-6	124164	36	44	0	73	19	15	1	26	9919
7.	38	089279-57-2	59761	42	62	1	74	21	14	0	29	9855
8.	*36	000111-53-5	9294	32	91	1	69	28	12	0	27	9865
9.	33	000000-00-0	21140	33	61	1	76	33	10	0	21	9741
10.	33	001447-26-3	120587	34	57	1	82	33	10	0	22	9805
11.	*33	032064-77-0	9333	25	36	1	80	32	10	1	26	9823
12.	33	053941-20-1	5333	33	46	2	73	35	10	0	22	9798
13.	33	006294-40-2	23641	37	44	2	99	35	10	0	22	9801
14.	*33	000000-00-0	675	29	72	3	99	35	10	0	29	9695
15.	28	005682-00-8	20532	34	56	2	68	39	8	0	22	9312
16.	25	004464-77-1	31629	34	64	2	70	42	7	0	25	9165

Peak 99



Scan 926 (19.776 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	92	70.85	146	95.90	85	122.95	169
44.80	166	76.95	70	98.95	128	123.95	102
52.95	8	77.80	169	101.80	54	124.95	22
54.85	104	79.95	74	107.90	102	128.80	63
56.95	54	80.95	33	108.90	6	135.90	114
62.90	5	82.80	13	110.95	119	150.05	21
64.95	110	83.90	188	111.95	45	150.95	1127
65.90	107	85.90	5	114.90	145	151.80	233
66.95	51	91.90	126	119.00	98	152.80	74
69.00	67	92.95	44	121.80	77	166.00	314
69.95	148	94.95	151	122.05	91	167.00	118

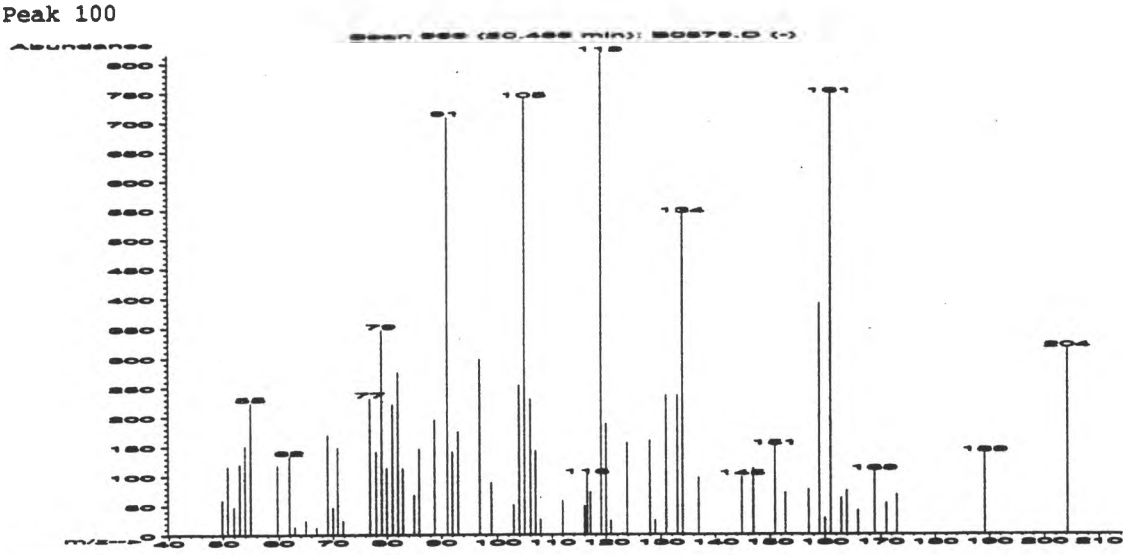
Scan 926 (19.776 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1,2-Benzenediol, 4-(1,1-dimethylethyl)-	166	C10H14O2	59
2.	CIS-1-TRIMETHYLSILYLHEPT-3-EN-1-YNE	166	C10H18Si	53
3.	2-Ethyl-1-(isopropylamino)-1-cyanobutene	166	C10H18N2	52
4.	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-te	151	C8H9NO2	49
5.	Ethanone, 1-(2-hydroxy-4-methoxyphenyl)-	166	C9H10O3	47
6.	Thieno[3,2-c]pyridine 5-Oxide Hemihydrat	151	C7H5NOS	43
7.	2(3H)-Benzoxazolethione	151	C7H5NOS	43
8.	P-FORMANISIDINE	151	C8H9NO2	43
9.	Thiazolo[5,4-d]pyrimidine, 7-methyl-	151	C6H5N3S	38
10.	1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	38
11.	1H-Isoindole-1,3(2H)-dione, 3a,4,7,7a-te	151	C8H9NO2	38
12.	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-	166	C9H10O3	35
13.	4-AMINO-1,2,3-BENZOTHIADIAZOLE	151	C6H5N3S	35
14.	Ethanone, 1-(2-hydroxy-5-methoxyphenyl)-	166	C9H10O3	35
15.	Silane, trimethylphenoxy-	166	C9H14OSi	33
16.	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-	166	C9H10O3	32
17.	1,2,4-Triazolo[4,3-a]pyridine-3(2H)-thio	151	C6H5N3S	32
18.	Benzaldehyde, 4-hydroxy-3-methoxy-	152	C8H8O3	32
19.	Ethanone, 1-(4-hydroxy-3-methoxyphenyl)-	166	C9H10O3	25
20.	4-(METHYLTHIO)ACETOPHENONE	166	C9H10OS	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	000098-29-3	125560	37	59	2	91	22	33	1	40	9778
2.	*53	060216-46-8	125585	37	56	1	99	30	28	0	39	9672
3.	*52	000000-00-0	19540	52	53	0	75	32	27	0	46	9775
4.	*49	001469-48-3	123801	35	51	0	91	40	23	4	43	9476
5.	*47	000552-41-0	19313	36	54	1	80	36	20	0	41	9629
6.	*43	086344-82-3	13021	44	60	2	82	44	18	0	40	9289
7.	*43	002382-96-9	13019	37	43	0	83	48	18	10	43	9290
8.	*43	023896-88-0	123799	33	43	2	82	44	18	0	39	7884
9.	*38	013316-06-8	13011	34	51	2	99	40	14	8	35	9257
10.	*38	002634-33-5	13018	31	60	2	99	39	14	0	33	9380
11.	*38	001469-48-3	13115	30	56	1	99	39	14	8	35	9457
12.	*35	000498-02-2	125553	35	62	0	51	51	11	0	41	9601
13.	*35	000000-00-0	13008	33	54	2	93	52	11	0	39	9174
14.	*35	000705-15-7	19315	36	62	1	63	53	11	13	40	9135
15.	*33	001529-17-5	125555	32	61	1	99	34	10	0	29	9623
16.	*32	000498-02-2	125551	29	58	1	47	50	9	0	33	9406
17.	*32	006952-68-7	13012	34	76	2	99	47	9	0	35	9262
18.	32	000121-33-5	13356	43	67	1	71	47	9	0	35	8015
19.	*25	000498-02-2	125550	30	57	0	47	51	7	0	33	9402
20.	*25	000000-00-0	19251	31	69	0	53	52	7	0	33	9543

Peak 100



Scan 969 (20.486 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.80	59	69.00	169	84.95	68	106.05	230
50.80	116	69.95	46	85.90	146	106.95	143
51.95	48	70.85	148	88.75	195	107.85	26
52.95	120	71.85	24	91.00	706	111.95	58
53.95	151	76.85	231	91.95	141	115.95	49
54.95	224	78.00	141	93.00	175	116.40	101
59.75	118	78.95	345	96.80	297	117.00	73
61.90	133	79.95	113	98.95	88	119.00	814
62.90	14	81.00	221	102.95	51	119.95	188
64.95	24	81.95	275	103.95	254	120.85	24
66.95	13	82.90	113	104.95	737	122.95	2

Scan 969 (20.486 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.80	156	157.05	76	204.20	313		
127.95	159	159.00	389				
128.95	25	160.00	28				
130.95	236	161.00	744				
133.00	236	162.90	62				
134.00	541	163.90	75				
136.90	97	165.90	41				
144.90	98	168.90	106				
146.95	112	171.05	53				
150.95	149	172.95	68				
152.80	71	189.15	137				

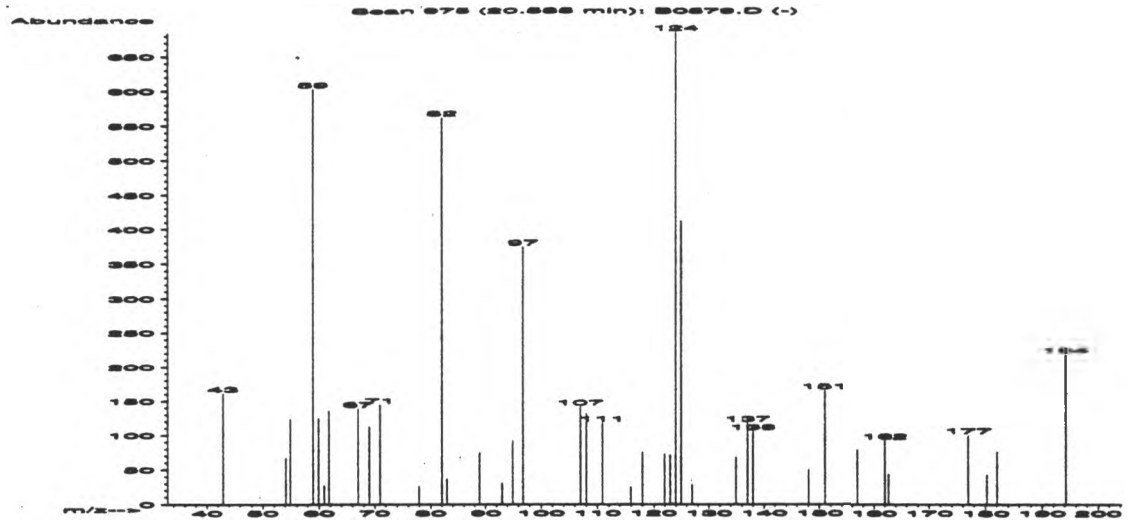
Scan 969 (20.486 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Naphthalene, 1,2,3,4,4a,7-hexahydro-1,6-	204	C15H24	46
2.	Acetonitrile, (3,5,5-trimethyl-2-cyclohe	161	C11H15N	27
3.	s-Triazolo[4,3-a]pyridine, 3,5,7-trimeth	161	C9H11N3	27
4.	3-PHENYL-4-METHYL-2-ISOXAZOLINE	161	C10H11NO	25
5.	2-METHYL-3-CIS-PROPENYLPYRAZINE	134	C8H10N2	22
6.	5H-5-METHYL-6,7-DIHYDROCYCLOPENTA(B)PYRA	134	C8H10N2	22
7.	1,4-Cyclohexadiene, 3-ethenyl-1,2-dimeth	134	C10H14	18
8.	P-MENTHA-1,5,8-TRIENE	134	C10H14	18
9.	.gamma.-Cadinene	204	C15H24	15
10.	Ethanone, 1-(2-methylphenyl)-	134	C9H10O	14
11.	trans-Chrysanthenyl acetate	194	C12H18O2	14
12.	Benzene, 1,3-diethyl-	134	C10H14	14
13.	Calarene	204	C15H24	12
14.	CYCLOHEPTANE, 1,3,6-TRIMETHYLENE-	134	C10H14	11
15.	2(1H)-Quinolinone, 1-hydroxy-	161	C9H7NO2	11
16.	Cycloheptane, 1,3,5-tris(methylene)-	134	C10H14	11
17.	Cycloheptane, 1,3,5-tris(methylene)-	134	C10H14	10
18.	4-METHYL-3-(2-PYRIDYL)-1,2,4-OXADIAZOLE	161	C8H7N3O	10
19.	Tricyclo[6.2.1.0(2,6)]undec-2(6)-ene	148	C11H16	10
20.	P-MENTHA-1,5,8-TRIENE	134	C10H14	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	016728-99-7	128733	66	65	0	88	43	20	12	47	8314
2.	*27	069697-21-8	17332	28	81	2	91	59	8	0	39	8196
3.	*27	004919-15-7	17230	35	97	3	92	60	8	0	39	7923
4.	*25	051067-04-0	17268	49	67	1	77	55	7	7	37	8101
5.	*22	000000-00-0	7338	34	73	1	99	64	5	0	39	7223
6.	*22	000000-00-0	7363	39	55	1	97	65	5	5	40	7195
7.	*18	062338-57-2	7463	51	61	1	97	68	3	17	45	6898
8.	*18	021195-59-5	7462	49	62	1	99	70	3	0	44	7022
9.	*15	039029-41-9	128720	59	78	2	162	72	2	0	51	7392
10.	*14	000577-16-2	121573	33	74	1	86	68	2	0	39	7051
11.	14	050764-55-1	31953	44	82	2	91	70	2	9	38	6802
12.	*14	000141-93-5	121643	46	51	0	70	69	2	11	40	6976
13.	12	017334-55-3	128758	46	93	2	90	61	2	8	37	7054
14.	*11	000000-00-0	7467	55	62	1	66	78	2	0	47	6610
15.	*11	000058-57-1	17192	37	65	0	91	78	2	10	43	5379
16.	*11	068284-24-2	121679	55	62	1	66	78	2	0	47	6610
17.	*10	068284-24-2	7466	47	72	2	83	78	1	0	40	6661
18.	*10	001455-84-1	17158	51	43	0	71	80	1	2	41	5345
19.	10	057496-70-5	12160	58	47	0	92	80	1	0	43	5848
20.	*10	021195-59-5	121678	33	69	0	66	77	1	0	41	6676

Peak 101



Scan 975 (20.585 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	161	82.00	560	121.95	73	162.00	91
54.05	67	82.90	37	122.95	71	162.65	43
54.85	123	88.90	74	123.95	684	176.95	99
58.90	602	93.00	31	124.95	412	180.30	42
59.90	124	94.95	92	126.90	28	182.05	75
60.90	27	96.80	374	134.90	68	194.15	218
61.75	135	106.95	141	137.00	117		
67.00	138	108.00	131	138.00	105		
69.00	112	110.90	117	148.05	49		
70.95	144	115.95	25	150.95	165		
77.95	26	118.00	75	156.95	78		

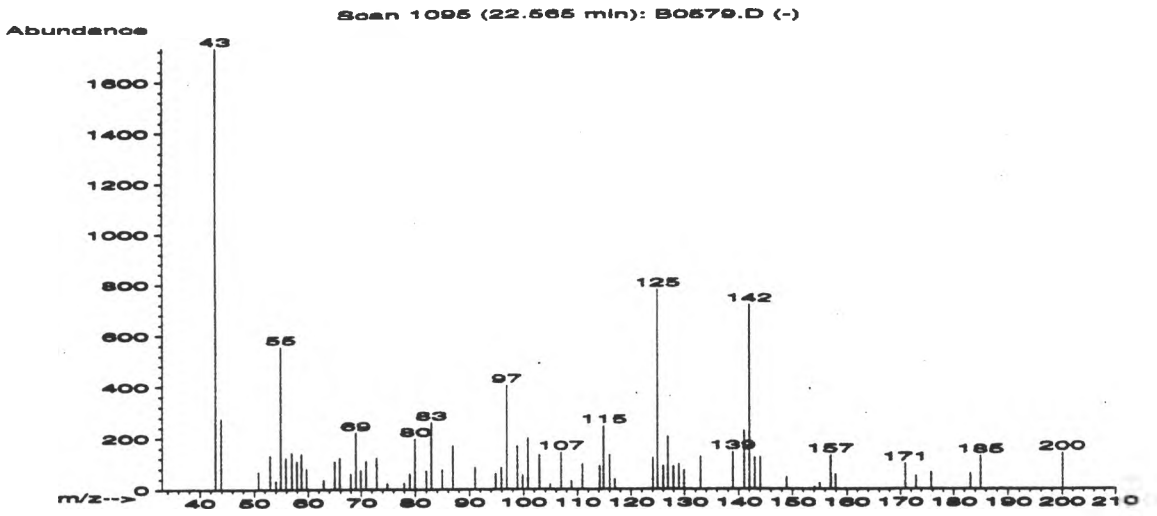
Scan 975 (20.585 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	4-tert-Butyl-1,1-dimethyl-1-sila-4-borac	182	C10H23BSi	25
2.	2-Cyclohexen-1-one, 4,4-dimethyl-	124	C8H12O	22
3.	5,5,9,9-TETRAMETHYLCYCLONON-2(CIS)-EN-1,	208	C13H20O2	12
4.	4-Cyclopropyl-1,2,4-trimethyl-4-silacycl	166	C10H18Si	10
5.	10,10-DIMETHYL-9-OXA-11-AZABICYCLO(6.2.1	181	C11H19NO	10
6.	[(E)-7-Hydroxy-3,7-dimethyl-6-oxo-2-octe	228	C12H20O4	10
7.	Benzoic acid, 4-hydroxy-3-methoxy-	168	C8H8O4	10
8.	ENDO-2-HYDROXY-5-KETOBORNANE	168	C10H16O2	8
9.	2-AZA-HEXAMETHYLTRICYCLO-(3.3.0.0)OCTAN-	207	C13H21NO	8
10.	Olealdehyde, dimethyl acetal	312	C20H40O2	8
11.	Undecanenitrile	167	C11H21N	7
12.	2-Acetyl-5-methylfuran	124	C7H8O2	7
13.	1-ISOPROPYL-4-METHYL-7-OXASPIRO(4.5)DECA	212	C13H24O2	7
14.	Isopulegone	152	C10H16O	7
15.	Mebutamate	232	C10H20N2O4	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*25	089555-74-8	26595	44	85	0	68	64	7	0	44	7127
2.	*22	001073-13-8	120410	38	66	0	67	64	5	0	39	7344
3.	12	058643-90-6	38549	38	95	1	151	60	2	0	28	7307
4.	10	080631-69-2	19550	36	100	2	91	58	1	0	18	8187
5.	10	055087-35-9	26159	49	71	1	89	66	1	4	35	6992
6.	10	000000-00-0	47539	33	96	1	87	65	1	0	21	6535
7.	10	000121-34-6	125716	43	91	1	97	66	1	0	35	4593
8.	8	059169-18-5	20474	35	97	1	72	69	1	0	22	6733
9.	8	000000-00-0	38028	40	81	1	95	69	1	0	29	6546
10.	8	015677-71-1	77791	41	118	3	280	68	1	0	29	6721
11.	7	002244-07-7	125667	35	94	1	54	79	1	0	22	6942
12.	* 7	001193-79-9	120362	31	83	1	74	76	1	0	26	6867
13.	7	057683-89-3	40449	38	110	3	81	76	1	0	27	4751
14.	7	029606-79-9	123984	35	63	1	55	80	1	0	21	4670
15.	7	000064-55-1	48947	37	87	0	48	75	1	0	25	3156

Peak 102



Scan 1095 (22.565 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	1732	62.90	37	79.95	196	100.85	199
43.90	275	64.95	107	82.00	72	102.95	134
50.80	68	65.90	122	82.90	260	104.95	20
52.95	132	67.95	60	84.90	76	106.95	143
54.00	33	68.95	219	86.90	170	108.90	31
54.95	555	69.90	74	91.00	83	110.90	97
55.90	122	70.90	109	94.85	61	114.15	90
56.95	143	72.85	122	95.95	83	114.90	246
57.90	109	74.85	23	96.95	404	116.00	134
58.75	138	77.95	24	98.85	168	116.95	39
59.75	80	78.95	61	99.85	56	124.05	121

Scan 1095 (22.565 min): B0579.D

Modified:subtracted clipped

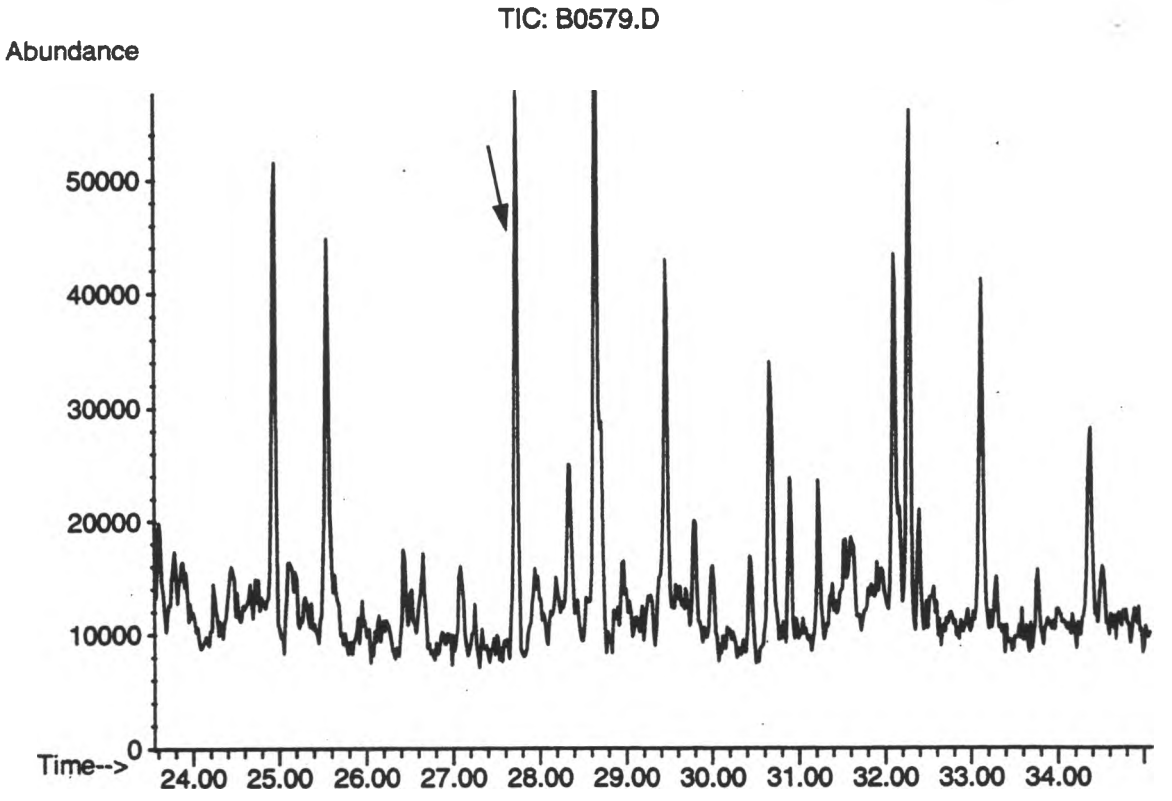
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
124.95	780	144.00	124	185.00	129		
126.00	90	148.95	46	200.05	140		
126.95	204	152.95	1				
127.95	88	154.10	9				
128.95	98	155.05	24				
129.95	72	157.00	132				
132.90	126	157.90	58				
138.90	144	170.95	99				
141.00	227	172.95	52				
142.00	718	175.80	65				
143.00	123	183.15	61				

Scan 1095 (22.565 min): B0579.D

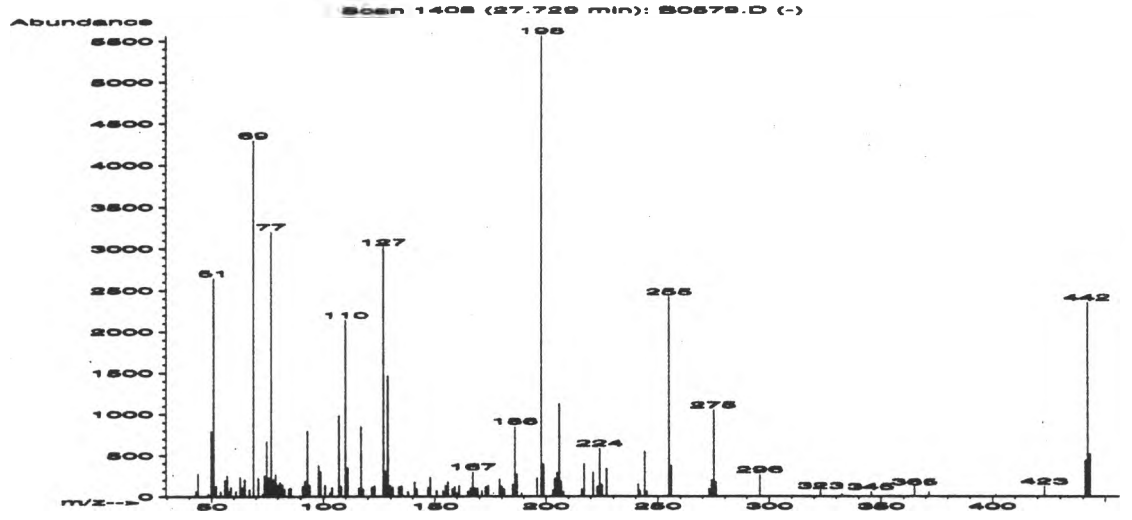
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Propanoic acid, 2,3-dichloro-, 1-methyle	184	C6H10Cl2O2	12
2.	1-Azabicyclo[2.2.2]octane, 4-methyl-	125	C8H15N	12
3.	1H-Indene-1-methanol, .alpha.-methyl-, a	202	C13H14O2	10
4.	2,3-EPOXY-2,6,6-TRIMETHYL-CYCLOHEPT-4-EN	168	C10H16O2	10
5.	3-Nonen-2-one	140	C9H16O	10
6.	2-ACETYL-1,4,5,6-TETRAHYDROPYRIDINE	125	C7H11NO	10
7.	Undecanoic acid, 11-amino-	201	C11H23NO2	10
8.	Isoxazole, 3,5-dimethyl-4-nitro-	142	C5H6N2O3	9
9.	1-BUTEN-2,4-DICARBONIC ACID, 2-METHYLEST	200	C10H16O4	9
10.	.alpha.-D-Glucopyranoside, methyl, tetra	362	C15H22O10	9
11.	CYCLOHEXENE, 1-ACETYL-2-(1-HYDROXYETHYL)	168	C10H16O2	7
12.	Ethanone, 1-(2-ethyl-4,4,6-trimethyl-1,3	198	C10H19BO3	7
13.	Borane, tributyl-	182	C12H27B	7
14.	1R-ACETAMIDO-4C-ACETOXY-5,6C-EPOXY-2C,3T	273	C12H19NO6	7
15.	Hexanoic acid, 2-acetyl-, ethyl ester	186	C10H18O3	7
16.	1-Hepten-1-ol, acetate	156	C9H16O2	7
17.	4(1H)-Pyrimidinone, 2-(methylthio)-	142	C5H6N2OS	7
18.	4H-Pyran-4-one, 5-hydroxy-2-(iodomethyl)	252	C6H5IO3	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	12	054774-99-1	27159	58	49	1	86	62	2	0	31	7497
2.*	12	045651-41-0	5040	33	74	3	99	63	2	0	35	7109
3.	10	063839-85-0	35659	43	40	1	84	75	1	9	38	6014
4.	10	058795-43-0	20451	37	62	0	44	63	1	0	25	7115
5.	10	014309-57-0	9329	41	61	2	62	63	1	0	29	7089
6.*	10	000000-00-0	5002	33	70	1	73	66	1	0	35	6994
7.	10	002432-99-7	35093	44	74	1	120	69	1	0	34	5980
8.*	9	001123-49-5	122587	32	60	1	55	74	1	8	35	6008
9.	9	000000-00-0	34570	42	63	0	16	80	1	0	33	3202
10.	9	000604-70-6	90586	56	75	0	90	80	1	0	36	3699
11.	7	000000-00-0	20391	33	57	1	44	74	1	0	22	6565
12.	7	074663-80-2	33763	33	90	2	52	71	1	0	20	6683
13.	7	000122-56-5	127032	39	62	1	54	72	1	0	29	6730
14.	7	000000-00-0	64547	35	70	0	23	78	1	0	25	3114
15.	7	001540-29-0	28370	49	69	2	59	78	1	0	27	2858
16.	7	035468-97-4	15371	38	48	2	157	80	1	0	29	3667
17.*	7	005751-20-2	122584	28	94	2	64	72	1	0	29	5857
18.	6	016065-34-2	56985	33	125	1	72	68	1	0	13	5526


TIC: B0579.D
Abundance
50000
40000
30000
20000
10000
0
Time-->
24.00
25.00
26.00
27.00
28.00
29.00
30.00
31.00
32.00
33.00
34.00

Peak 103



Scan 1408 (27.729 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	64	58.75	111	75.95	231	91.00	121
43.90	278	60.90	65	76.95	3199	91.90	185
48.45	36	62.90	239	77.95	209	93.00	797
49.80	795	63.90	107	78.95	271	94.00	138
50.80	2641	65.00	206	79.95	138	97.80	374
51.90	131	67.00	83	80.95	168	98.80	301
53.95	58	68.90	4295	81.95	138	100.80	136
54.95	10	70.95	225	82.90	88	102.90	44
55.95	199	72.90	31	84.90	87	103.80	107
56.95	252	73.90	253	85.50	101	105.00	1
57.75	66	74.95	674	85.75	100	106.95	984

Scan 1408 (27.729 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.90	121	128.95	1464	147.95	234	167.00	298
109.90	2136	129.80	129	150.80	70	167.90	99
110.95	349	130.95	111	153.80	69	169.00	99
114.90	5	132.90	1	154.95	132	171.05	62
115.90	97	133.75	119	155.95	178	172.80	115
116.90	848	134.95	126	157.90	88	173.80	131
117.90	85	135.75	13	158.90	112	178.95	210
121.80	110	137.90	59	159.75	41	179.95	120
122.95	131	140.95	173	160.90	133	181.05	85
126.95	3013	141.90	91	164.90	60	184.90	145
127.95	303	147.00	106	166.00	95	185.90	851
m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
186.90	269	215.90	86	254.95	2417	371.45	51
189.00	39	217.00	393	255.95	370	422.95	121
195.95	221	220.95	290	272.80	83	441.00	431
197.95	5557	222.95	117	273.95	194	442.00	2351
198.95	390	223.95	583	274.95	1049	443.00	515
203.05	70	224.95	142	275.95	176		
203.95	220	226.95	334	295.80	263		
205.05	286	241.15	147	322.95	68		
205.95	1126	242.00	69	332.55	33		
206.80	185	244.00	548	345.55	55		
207.90	61	245.05	59	364.90	112		

Scan 1408 (27.729 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

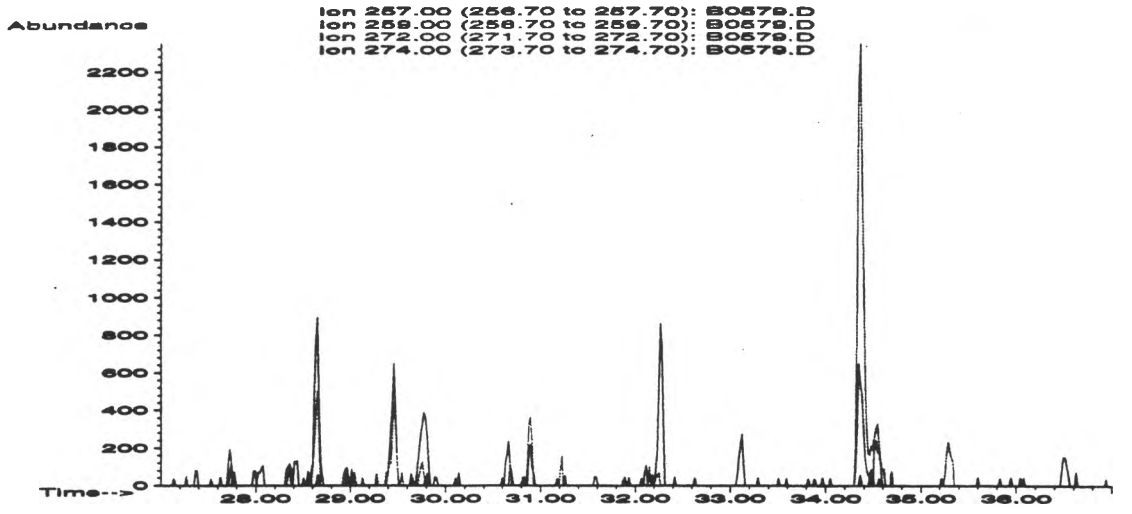
	Name	MolWt	Formula	Qual
1.	Phosphine, bis(pentafluorophenyl)phenyl-	442	C18H5F10P	99
2.	BIS(TRIFLUOROMETHYL)THIONE S-OXIDE	198	C3F6OS	27
3.	7,7-Ethylenedioxy-4a-(2-methoxyethyl)-ci	255	C14H25NO3	10
4.	Hydrazine, (pentafluorophenyl)-	198	C6H3F5N2	10
5.	5-NITRO-1-METHYLPYRAZOLE	127	C4H5N3O2	10
6.	3-NITRO-4-METHYLPYRAZOLE	127	C4H5N3O2	10
7.	3-NITRO-4-METHYLPYRAZOLE	127	C4H5N3O2	10
8.	N,2,3-TRIMETHYL-2-BUTENOIC ACID AMIDE	127	C7H13NO	10
9.	Benzoic-D5 acid	122	C7HD5O2	10
10.	Phosphorocyanidothioic difluoride	127	CF2NPS	10
11.	Hydrazine, (pentafluorophenyl)-	198	C6H3F5N2	9
12.	Benzenamine, 4,4'-methylenebis-	198	C13H14N2	9
13.	Benzenamine, 4,4'-methylenebis-	198	C13H14N2	9
14.	5-NITROTHIENO(3,2-D)THIAZOLE	186	C5H2N2O2S2	9
15.	IODOHEPTAFLUOROPROPANE	296	C3F7I	9
16.	2-Piperidineacetic acid, 1-acetyl-6-[1-(	299	C15H25NO5	7
17.	Pyridine, 4-(4-dimethylaminophenyl)-	198	C13H14N2	7
18.	Dibenzofuran, 2-methoxy-	198	C13H10O2	7
19.	Benzene, 1-methyl-2-(4-methylphenoxy)-	198	C14H14O	7
20.	2-Propen-1-one, 3-(2-furanyl)-1-phenyl-	198	C13H10O2	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*99	005074-71-5	136554	148	46	0	88	27	80	6	99	8424
2.	*27	087108-79-0	33441	36	106	2	79	56	8	0	39	7995
3.	10	080595-01-3	58501	33	57	2	99	64	1	0	22	6815
4.	*10	000828-73-9	33466	33	73	1	70	76	1	13	40	6750
5.	*10	054210-33-2	5488	37	84	0	54	78	1	0	41	4177
6.	*10	038858-90-1	120655	33	67	1	54	78	1	0	39	4199
7.	*10	038858-90-1	5485	34	61	2	49	78	1	0	39	4199
8.	*10	000000-00-0	5576	30	66	1	64	67	1	1	30	5972
9.	*10	000000-00-0	4333	36	50	2	42	78	1	0	41	4175
10.	*10	028314-61-6	5475	38	43	1	77	67	1	0	35	5958
11.	* 9	000828-73-9	128123	36	97	3	93	75	1	0	35	6781
12.	* 9	000101-77-9	128235	34	93	2	84	78	1	0	35	6326
13.	* 9	000101-77-9	34057	39	87	2	93	78	1	0	33	6326
14.	* 9	066646-12-6	28105	34	68	1	77	78	1	18	36	4889
15.	* 9	000000-00-0	72195	42	88	2	54	72	1	5	35	5892
16.	7	054984-46-2	73477	38	96	1	83	78	1	0	29	6326
17.	* 7	001137-80-0	34064	28	102	2	91	75	1	0	27	6763
18.	* 7	020357-70-4	34029	28	103	2	97	72	1	0	27	7030
19.	* 7	003402-72-0	34110	29	97	3	99	78	1	0	27	6326
20.	* 7	000717-21-5	128220	29	97	3	94	78	1	0	29	6326

Notes on P&G BKME Effluents

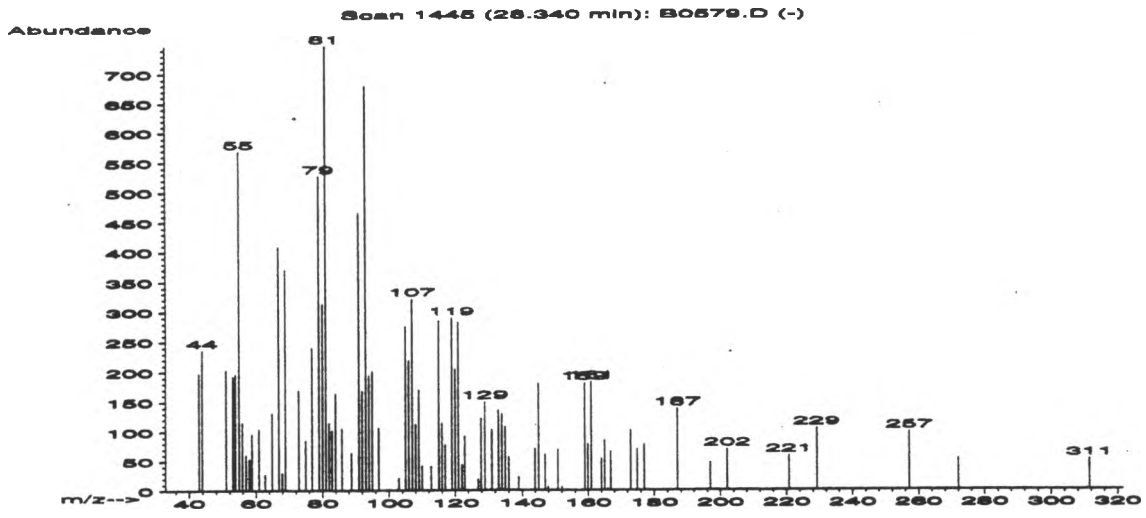
Terpenes

Easy to observe in B0579.D



Ions 257,279,272,274 are characteristic of diterpenes and used in trace above to show diterpenes in B0579.

Peak 104



Scan 1445 (28.340 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	197	62.75	27	81.95	114	102.85	21
43.90	236	64.95	131	82.90	102	104.95	275
50.95	203	67.00	408	83.95	163	105.95	218
52.95	192	67.95	30	85.90	105	107.00	321
53.80	196	68.95	369	88.75	64	107.95	112
54.95	569	72.95	169	91.00	466	108.90	169
55.95	115	74.95	85	91.95	168	109.90	42
56.95	60	76.95	240	93.00	679	112.65	41
58.00	53	78.95	527	94.05	194	115.00	284
58.75	96	80.05	312	94.95	201	116.00	114
60.90	104	81.00	746	96.95	106	116.95	78

Scan 1445 (28.340 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.00	289	134.95	108	161.00	183	220.80	59
119.95	204	135.95	57	164.00	54	229.20	105
120.95	282	138.90	23	165.00	85	257.20	99
122.00	44	143.90	71	166.00	2	272.05	53
122.90	92	144.95	180	166.90	66	311.50	52
126.95	19	146.95	61	173.05	102		
127.80	122	147.95	6	174.95	70		
128.95	150	150.80	70	177.05	78		
131.00	103	152.00	6	187.00	138		
133.00	136	158.90	181	196.80	47		
133.90	130	159.90	79	202.05	70		

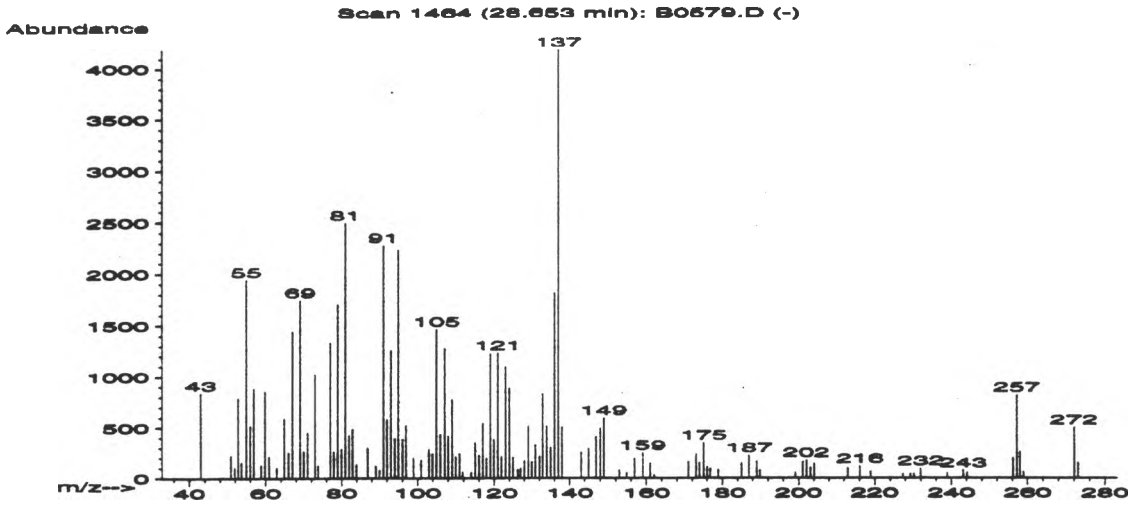
Scan 1445 (28.340 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Bicyclo[2.2.1]heptane, 2,2-dimethyl-3-me	136	C10H16	70
2.	6-Hexadecen-4-yne, (E)-	220	C16H28	35
3.	Cembrene	272	C20H32	30
4.	2-Pentadecen-4-yne, (Z)-	206	C15H26	27
5.	2-Dodecen-4-yne, (Z)-	164	C12H20	27
6.	2-METHYL-N-PHENYL-3-BUTENOIC ACID AMIDE	175	C11H13NO	25
7.	1,3,7-OCTATRIENE, 3,7-DIMETHYL-	136	C10H16	25
8.	1,3,6-Octatriene, 3,7-dimethyl-, (E)-	136	C10H16	25
9.	2-Cyclohexylmethylenecyclopropane	136	C10H16	22
10.	1,3,6-Heptatriene, 2,5,5-trimethyl-	136	C10H16	18
11.	1,4,6-HEPTATRIENE, 3,3,6-TRIMETHYL-	136	C10H16	18
12.	(+-)-trans-1-(1-Methylethenyl)-2-(2-meth	136	C10H16	18
13.	Camphene	136	C10H16	14
14.	1.ALPHA.,5,8-TRIMETHYL-TETRACYCLO[5.3.1.	202	C14H18O	11
15.	4-Tridecen-6-yne, (E)-	178	C13H22	10
16.	5,8,11-Heptadecatrienoic acid, methyl es	278	C18H30O2	10
17.	1,5-Hexadiene, 2,5-dimethyl-3-methylene-	122	C9H14	10
18.	.ALPHA.-PINENE, (-)-	136	C10H16	10
19.	CYCLOPENTANE, 1-METHYLEN-2-VINYL-	108	C8H12	10
20.	Cembrene	272	C20H32	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*70	005794-03-6	8150	79	35	0	79	63	41	0	93	6614
2.	35	074744-52-8	44082	59	80	3	220	55	11	0	39	8591
3.	*30	001898-13-1	64438	69	87	0	50	61	9	24	59	8984
4.	27	074646-33-6	128882	61	74	3	136	57	8	0	39	6652
5.	27	074744-37-9	18708	60	55	3	215	57	8	0	39	6701
6.	*25	000000-00-0	23450	63	47	0	89	63	7	18	47	6313
7.	*25	000502-99-8	8064	47	66	0	91	64	7	0	44	6891
8.	*25	003779-61-1	121952	50	66	0	73	64	7	0	46	7002
9.	*22	057497-09-3	8141	36	69	0	82	65	5	0	41	8629
10.	*18	029548-02-5	8069	44	71	0	66	69	3	0	44	6575
11.	*18	000000-00-0	8072	44	71	0	66	69	3	0	44	6575
12.	*18	080082-35-5	8076	47	45	0	91	68	3	0	44	6174
13.	*14	000079-92-5	122047	62	54	1	91	68	2	11	40	6872
14.	*11	058537-28-3	35759	33	56	0	38	76	2	18	43	3908
15.	10	074744-43-7	24942	56	66	0	70	76	1	12	41	6700
16.	10	022117-08-4	66505	70	103	0	54	73	1	0	42	6443
17.	*10	059131-13-4	4462	48	57	0	62	77	1	24	41	5870
18.	*10	000080-56-8	122067	34	68	0	91	73	1	0	41	6281
19.	*10	006196-78-7	118756	35	72	0	61	75	1	0	41	6218
20.	*10	001898-13-1	132281	47	100	0	31	78	1	22	43	9010

Peak 80



Scan 1464 (28.653 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	837	62.90	102	78.95	1707	93.00	1257
50.90	222	64.90	594	79.95	288	94.00	391
51.95	104	66.00	256	80.95	2495	94.95	2235
52.85	790	67.00	1445	81.95	424	96.05	384
53.70	153	69.00	1748	82.90	488	96.95	515
54.95	1945	69.95	268	83.95	134	98.95	197
55.95	518	70.95	452	86.90	298	100.95	175
56.95	885	72.95	1022	89.00	118	102.95	286
58.75	130	73.80	125	90.00	76	103.95	239
59.75	853	76.95	1332	91.00	2277	104.95	1462
60.90	213	77.95	264	92.00	578	105.95	431

Scan 1464 (28.653 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.05	1278	119.00	1226	129.95	160	146.95	411
108.00	417	119.95	380	130.95	331	148.05	490
109.00	776	120.95	1231	132.05	217	148.95	595
109.90	210	121.90	212	132.90	832	152.95	78
110.90	244	122.95	1098	134.00	514	154.90	54
111.75	60	123.95	887	135.00	305	156.95	196
114.00	57	124.95	208	136.00	1815	159.00	250
115.00	348	126.20	83	137.00	4185	160.95	147
116.00	225	126.95	100	138.00	508	162.00	31
117.00	543	127.95	173	143.00	258	170.95	161
118.00	197	129.05	513	144.95	291	173.05	238

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
173.95	155	202.05	178	243.15	75		
175.05	348	203.05	105	244.15	52		
175.95	112	204.05	145	256.20	202		
176.80	93	213.00	102	257.20	822		
178.95	78	216.15	118	258.00	261		
185.00	146	218.90	63	259.00	57		
187.00	226	227.30	40	272.05	503		
189.00	164	229.20	41	273.05	150		
189.90	79	230.20	42				
199.05	54	231.95	97				
201.05	164	238.90	50				

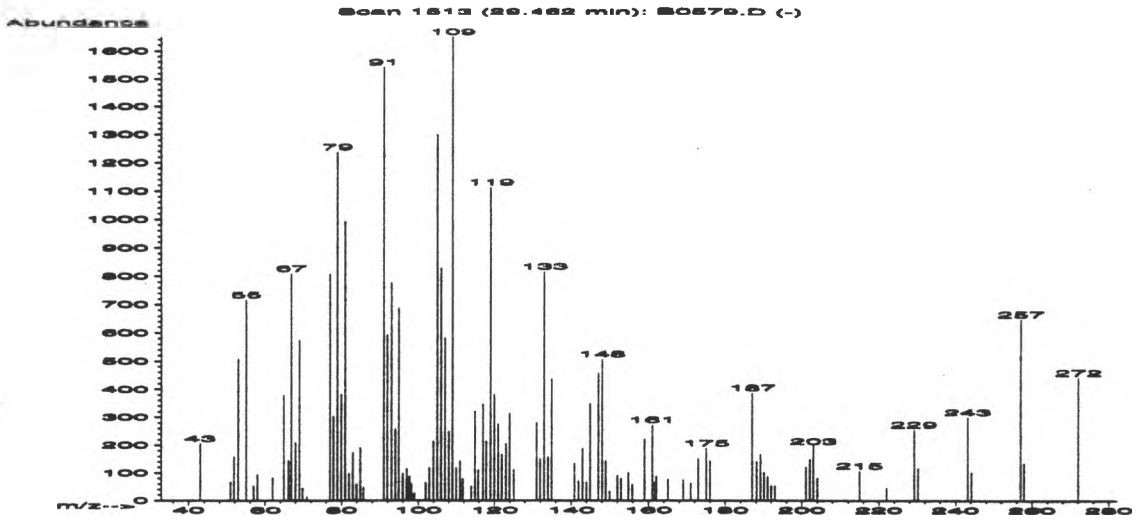
Scan 1464 (28.653 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Sandaracopimaradiene	272	C20H32	95
2.	2-AMINO-4,5,6,7-D4-BENZIMIDAOLE	133	C7H3D4N3	42
3.	1-Buten-1-ol, 2-methyl-4-(2,6,6-trimethy	236	C15H24O2	35
4.	Naphthalene, 2-butyldecahydro-	194	C14H26	35
5.	Naphthalene, 2-butyldecahydro-	194	C14H26	35
6.	BICYCLO[3.3.1]NON-1-BROMO-3-ONE	216	C9H13BrO	30
7.	BICYCLO[3.3.1]NON-1-BROMO-3-ONE	216	C9H13BrO	30
8.	Phenol, 4-amino-2,5-dimethyl-	137	C8H11NO	27
9.	Benzene, 1-methyl-4-nitro-	137	C7H7NO2	22
10.	(3.alpha.,6a.alpha.,6b.alpha.,9.beta.,12	272	C18H24O2	22
11.	3-METHYLENE-BICYCLO[4.3.0]NONANE	136	C10H16	18
12.	P-MENTH-2-EN-9-OL, TRANS	154	C10H18O	14
13.	Cyclodecene, 3-bromo-	216	C10H17Br	14
14.	Naphthalene, 2-butyldecahydro-	194	C14H26	14
15.	Benzoic acid, 4-methyl-	136	C8H8O2	11
16.	Trachylobane	272	C20H32	11
17.	Benzeneacetic acid, .alpha.-hydroxy-4-me	196	C10H12O4	10
18.	Acetic acid, thiocyanato-, 1,7,7-trimeth	253	C13H19NO2S	10
19.	Benzoic acid, 3-methyl-	136	C8H8O2	10
20.	ENDOBORNYL ACETATE	196	C12H20O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*95	001686-56-2	132292	96	71	0	58	43	72	0	96	9724
2.	*42	000000-00-0	7100	67	30	0	71	56	17	0	64	8157
3.	35	021730-91-6	50874	43	72	0	92	53	11	12	41	8616
4.	35	006305-52-8	127890	46	67	0	69	54	11	3	41	8719
5.	35	006305-52-8	32163	46	72	0	73	55	11	0	39	8652
6.	*30	066077-98-3	129423	57	62	0	82	56	9	0	49	8361
7.	*30	066077-98-3	41754	50	38	0	70	58	9	0	46	8233
8.	*27	003096-71-7	8316	45	65	2	99	57	8	13	38	8031
9.	*22	000099-99-0	122130	37	72	3	145	65	5	0	39	7668
10.	*22	071370-28-0	64349	60	127	2	51	65	5	0	41	8480
11.	*18	000000-00-0	8180	57	64	2	39	68	3	0	49	5500
12.	14	000000-00-0	14674	78	51	1	53	68	2	0	41	5439
13.	*14	056325-56-5	41810	45	80	0	57	68	2	4	40	6612
14.	14	006305-52-8	127889	60	66	0	63	68	2	0	43	8649
15.	*11	000099-94-5	121829	46	38	0	52	77	2	0	44	4393
16.	*11	005282-35-9	64471	50	94	0	17	79	2	0	46	6317
17.	10	013305-14-1	32700	43	70	0	67	71	1	0	39	7429
18.	10	000115-31-1	57663	57	75	1	36	75	1	22	39	5797
19.	*10	000099-04-7	121824	44	59	2	68	75	1	0	39	4570
20.	10	000076-49-3	128023	44	70	0	34	76	1	4	39	5317

Peak 81



Scan 1513 (29.462 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	206	68.00	209	83.90	60	98.20	61
50.85	67	69.00	572	84.90	191	98.95	26
51.80	160	69.85	45	85.75	47	101.95	65
52.90	508	70.95	13	91.00	1539	102.90	118
54.95	716	76.95	807	91.90	590	103.95	214
56.95	52	77.95	303	93.00	775	104.95	1296
57.90	94	78.95	1236	94.00	257	105.95	826
61.90	82	79.95	381	94.95	685	107.00	580
64.85	379	80.95	991	95.95	98	108.00	249
66.15	145	81.95	97	96.95	115	108.90	1649
66.90	808	82.95	173	97.70	88	109.95	118

Scan 1513 (29.462 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.00	144	123.00	205	143.00	187	159.00	221
111.75	79	123.95	314	144.00	66	161.00	272
113.90	51	125.00	111	144.95	348	161.75	66
114.90	321	131.00	280	147.05	456	162.00	87
115.75	110	131.95	151	148.05	505	165.00	77
117.00	347	133.00	814	148.95	144	169.00	75
117.90	214	134.00	157	150.00	33	170.95	62
119.00	1109	134.90	435	152.05	91	172.95	151
119.95	380	136.90	3	152.95	79	175.05	188
120.95	275	140.90	134	154.80	102	176.05	143
121.95	167	141.95	71	155.80	58	187.00	386

Scan 1513 (29.462 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
188.15	141	221.95	46				
189.15	167	229.20	255				
190.15	102	230.20	117				
191.00	86	243.15	300				
192.00	52	244.15	102				
193.00	53	257.05	647				
201.05	120	258.00	134				
202.05	149	272.05	441				
203.05	196						
204.05	81						
215.00	108						

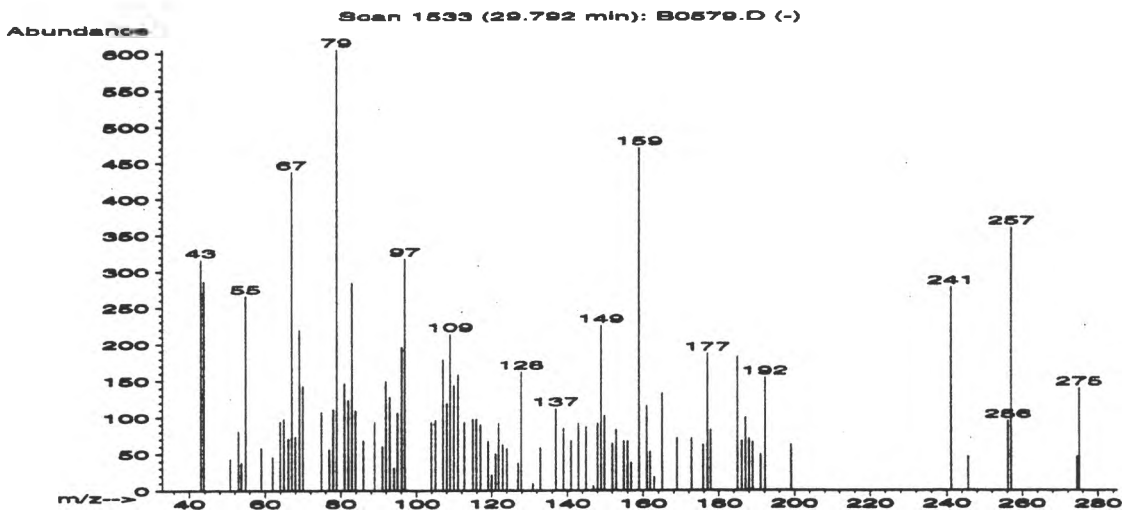
Scan 1513 (29.462 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	trans-Caryophyllene	204	C15H24	38
2.	1-Phenyl-2-buten-1-ol	148	C10H12O	15
3.	8-ETHYLCYCLO-OCTA-2,4,6-TRIENONE	148	C10H12O	14
4.	exo-4-Methylbicyclo[3.2.1]octan-3-ene	122	C9H14	11
5.	trans-Caryophyllene	204	C15H24	11
6.	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	11
7.	3-Tetradecen-5-yne, (E)-	192	C14H24	11
8.	3-Tetradecen-5-yne, (Z)-	192	C14H24	11
9.	Bicyclo[2.2.1]hept-2-en-7-ol	110	C7H10O	11
10.	N-(METHYL-D2)-ANILINE	107	C7H7D2N	11
11.	EXO-BICYCLO[4.1.0]HEPT-3-EN-7-ISOCYANATE	135	C8H9NO	10
12.	Phenol, 4-methoxy-	124	C7H8O2	10
13.	2-Cyclopenten-1-one, 3,4,5-trimethyl-	124	C8H12O	10
14.	2-Pentadecen-4-yne, (Z)-	206	C15H26	10
15.	Silane, chloroethylmethyl-	108	C3H9ClSi	10
16.	3,5-Heptadien-2-one, 6-methyl-, (E)-	124	C8H12O	10
17.	Cyclohexane, 1,2,4-triethenyl-	162	C12H18	10
18.	Mandelonitrile	133	C8H7NO	10
19.	CYCLOHEXANE, 1-CIS-2-TRANS-4-CIS-TRIVINY	162	C12H18	10
20.	(Bicyclo[4.1.0]hept-3-en-endo-7-yl)isocy	135	C8H9NO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	000087-44-5	128689	84	60	0	56	61	14	47	74	6088
2.	*15	000000-00-0	12028	62	65	1	50	79	2	0	56	5354
3.	*14	061775-57-3	12053	34	37	0	84	70	2	0	41	5069
4.	*11	078965-86-3	4484	34	63	0	52	80	2	10	43	4324
5.	*11	000087-44-5	128690	63	86	1	66	72	2	0	44	7249
6.	*11	000122-03-2	123389	55	62	1	55	77	2	0	49	5800
7.	*11	074744-44-8	31088	45	84	0	67	71	2	0	44	4900
8.	*11	074663-68-6	31087	46	83	0	74	76	2	0	44	4837
9.	*11	053783-87-2	2208	48	80	2	60	80	2	0	46	6062
10.	*11	056805-04-0	1829	52	63	2	76	77	2	0	44	6530
11.	*10	090013-14-2	7585	47	50	1	55	71	1	0	39	5154
12.	*10	000150-76-5	120386	44	49	0	71	80	1	5	40	5785
13.	*10	055683-21-1	120406	33	53	0	77	77	1	0	41	6260
14.	10	074646-33-6	37737	43	86	0	50	79	1	0	39	4738
15.	*10	006374-21-6	1855	46	66	1	74	77	1	0	40	5159
16.	*10	016647-04-4	4765	45	52	1	76	77	1	0	40	6604
17.	10	002855-27-8	17867	46	66	0	48	80	1	0	39	6236
18.	*10	000532-28-5	7120	43	70	1	59	78	1	0	39	4808
19.	10	000000-00-0	17865	46	66	0	48	80	1	0	39	6236
20.	*10	085156-51-0	7582	33	48	0	72	76	1	0	41	5063

Peak 105



Scan 1533 (29.792 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	316	66.00	71	82.90	284	103.95	93
43.75	286	66.95	438	83.90	109	105.00	96
50.80	43	67.95	73	85.90	68	107.00	179
52.95	81	69.00	219	88.90	93	108.00	119
53.75	38	69.95	143	90.95	60	108.90	213
54.85	266	74.95	107	91.90	149	109.90	144
55.90	1	76.95	56	92.95	128	111.00	158
58.95	58	77.95	111	94.00	31	112.75	93
61.90	46	78.95	605	94.95	106	114.95	97
63.90	94	80.95	146	96.05	195	115.90	97
64.95	97	81.95	123	96.95	317	117.00	90

Scan 1533 (29.792 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.00	67	136.95	112	154.95	68	176.95	187
120.00	21	139.00	85	155.95	68	177.80	83
120.95	50	140.95	68	156.95	38	184.90	183
121.85	92	142.95	92	159.00	470	186.00	68
122.95	62	144.95	87	161.00	116	187.00	100
124.05	57	146.95	6	161.90	53	188.00	71
124.95	1	148.05	92	162.90	18	188.90	66
126.95	37	148.95	225	164.90	133	191.00	49
127.80	162	149.95	102	168.90	72	192.15	154
130.95	9	151.95	64	172.70	71	199.05	62
132.90	58	152.95	84	175.80	62	241.15	278

Scan 1533 (29.792 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
245.55	46						
256.20	95						
257.05	360						
274.45	46						
275.05	140						

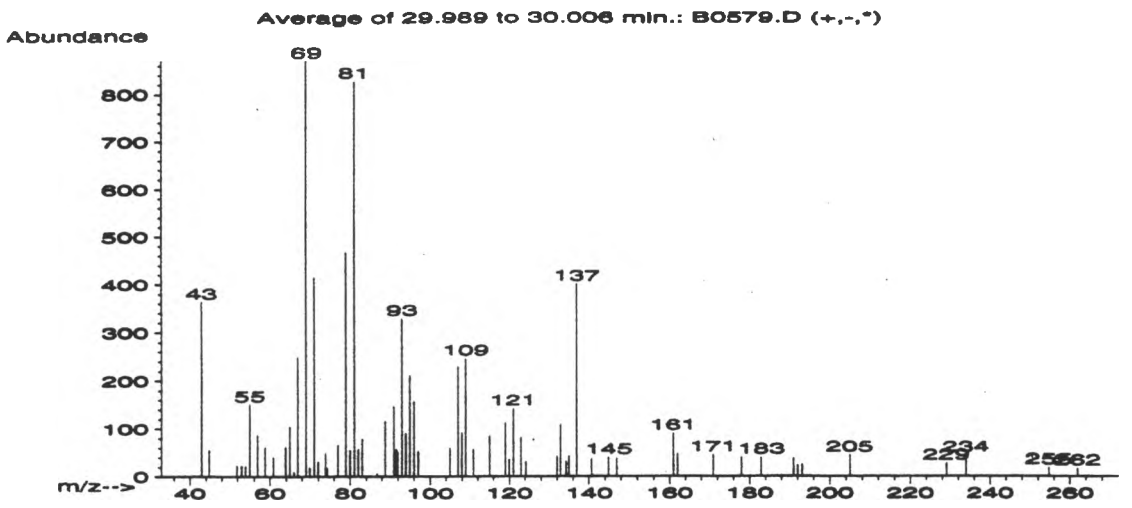
Scan 1533 (29.792 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	4-Tridecen-6-yne, (Z)-	178	C13H22	11
2.	3-Amino-5-chloro-1-methyl-2(1H)-pyrazino	159	C5H6ClN3O	10
3.	4-Quinolinol, 2-methyl-	159	C10H9NO	10
4.	1-METHYL-4-AMINO-5-CHLORO-6-OXO-(1H)-PYR	159	C5H6ClN3O	9
5.	(3aRS,6SR,7aSR)-6-Hydroxy-3a-phenyl-3a,6	229	C14H15NO2	9
6.	ANILINE, N-(1,3-BUTADIENYL)-N-METHYL-	159	C11H13N	9
7.	1H-Indene, 2,3-dihydro-1,1,5,6-tetrameth	174	C13H18	9
8.	5-Pentadecen-7-yne, (Z)-	206	C15H26	9
9.	6-Tridecen-4-yne, (E)-	178	C13H22	9
10.	4-Tridecen-6-yne, (E)-	178	C13H22	9
11.	9-ARISTOLEN-1.ALPHA.-OL	220	C15H24O	9
12.	4-Hexadecen-6-yne, (E)-	220	C16H28	9
13.	4-ISOPROPYL-2,6,7-TRIOXA-1-PHOSPHABICYCL	192	C7H13O4P	9
14.	3-(CYCLOHEX-3'-EN-YL)PROPIONALDEHYDE	138	C9H14O	9
15.	Oxazole, 5-methyl-2-phenyl-	159	C10H9NO	7
16.	1(2H)-Isoquinolinone, 2-methyl-	159	C10H9NO	7
17.	6-(3-METHYL-3-CYCLOHEXENYL)-2-METHYL-2,6	220	C15H24O	7
18.	4-Isopropyl-6-methyl-1,2,3,4-tetrahydron	202	C14H18O	7
19.	4-ISOPROPYL-2,6,7-TRIOXA-1-PHOSPHABICYCL	192	C7H13O4P	7
20.	6-Tridecen-4-yne, (Z)-	178	C13H22	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*11	074744-42-6	24941	53	69	2	99	77	2	0	47	6108
2.	*10	087486-43-9	16364	33	37	0	59	71	1	0	41	4745
3.	*10	000607-67-0	16468	46	71	1	54	77	1	0	40	4745
4.	* 9	017254-80-7	16366	32	88	0	55	76	1	0	33	5054
5.	9	086983-23-5	48020	42	91	0	52	73	1	0	33	4963
6.	* 9	000000-00-0	16518	34	83	2	75	77	1	0	35	4745
7.	9	000942-43-8	23278	50	69	1	75	77	1	0	31	4745
8.	9	074744-50-6	37740	48	86	2	84	77	1	12	32	6108
9.	* 9	074744-46-0	24940	34	77	2	99	77	1	0	35	6108
10.	* 9	074744-43-7	24942	40	87	2	87	77	1	0	33	6108
11.	9	034143-95-8	44041	45	126	3	70	76	1	0	31	4778
12.	9	074744-51-7	44081	57	89	2	70	77	1	0	36	6108
13.	* 9	051052-72-3	30541	33	101	3	113	72	1	2	32	6303
14.	9	060210-93-7	8636	44	52	1	70	77	1	4	35	6108
15.	* 7	005221-67-0	16490	28	73	1	69	77	1	0	27	4745
16.	* 7	004594-71-2	16486	32	78	1	74	77	1	0	29	4745
17.	7	018681-09-9	44066	39	118	3	98	72	1	0	28	7214
18.	7	057494-10-7	35725	35	45	1	55	77	1	0	25	4745
19.	* 7	051052-72-3	127670	40	94	2	110	72	1	0	25	6303
20.	* 7	074744-45-9	24939	30	72	1	73	77	1	2	29	6108

Peak 106



Average of 29.989 to 30.006 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	363	65.95	10	81.00	827	95.95	157
44.80	55	66.95	248	81.95	57	97.00	52
51.80	23	69.00	870	82.95	78	104.95	59
52.95	23	69.85	19	86.80	6	106.95	229
53.95	22	70.95	414	88.80	116	107.95	91
54.95	151	71.95	31	91.00	146	108.95	245
56.95	87	73.85	48	91.65	57	110.90	57
58.75	61	74.20	18	91.95	51	115.00	84
60.90	41	76.95	66	93.00	328	119.00	112
63.90	62	78.95	466	94.00	90	119.95	36
64.95	104	80.00	55	94.95	210	120.95	142

Average of 29.989 to 30.006 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
122.95	82	162.00	47	261.90	17		
124.20	31	170.95	45				
131.95	42	177.95	40				
132.90	108	182.90	40				
134.25	31	191.00	38				
134.95	43	192.00	24				
136.95	400	193.15	25				
140.75	37	204.95	45				
144.95	40	229.05	28				
146.95	38	233.90	44				
160.95	90	254.70	19				

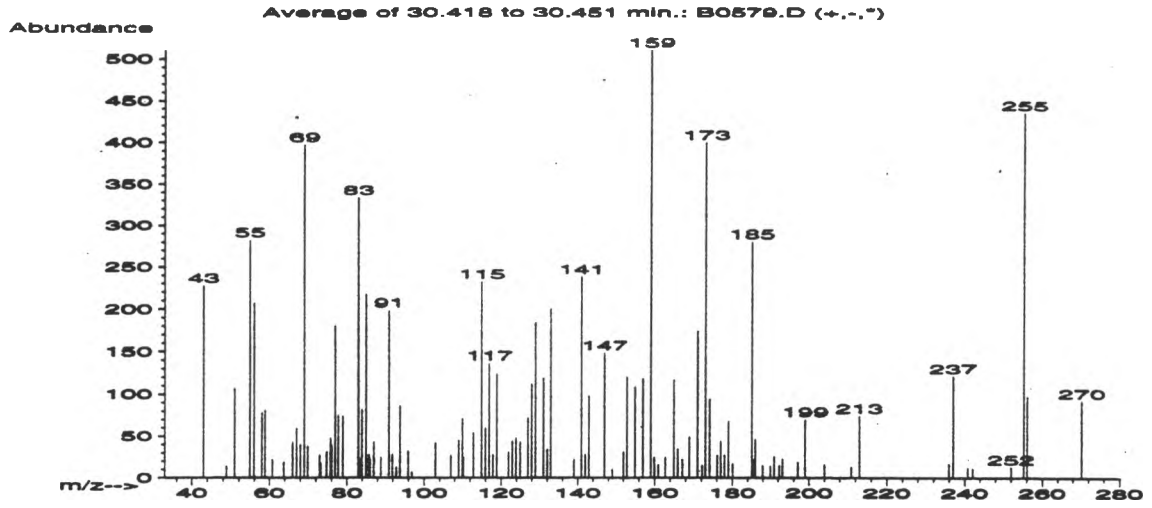
Average of 29.989 to 30.006 min.: B0579.D
Converted from RTE data file: >B0579:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	40
2.	2,6,10,15,19,23-HEXAMETHYL-2,6,10,14,18,	410	C30H50	40
3.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	37
4.	Cyclopentanecarboxylic acid, 3-methylene	262	C17H26O2	32
5.	Farnesol	222	C15H26O	32
6.	d-Nerolidol	222	C15H26O	25
7.	Grosheimine	262	C15H18O4	25
8.	Nerolidol	222	C15H26O	25
9.	NEROLIDOL ISOMER	222	C15H26O	25
10.	Farnesol	222	C15H26O	22
11.	1,7-Octadien-3-one, 2-methyl-6-methylene	148	C10H12O	16
12.	d-Nerolidol	222	C15H26O	16
13.	Naphthalene, 1-(1,1-dimethylethyl)decahy	194	C14H26	12
14.	.beta.-Farnesene	204	C15H24	12
15.	2(5H)-Furanone, 5-(2-furanylmethyl)-5-me	178	C10H10O3	10
16.	Cyclohexene, 3-(2-propynyl)-	120	C9H12	10
17.	Cyclopentane, 1-methyl-2-methylene-	96	C7H12	10
18.	Cyclohexene, 4-methyl-	96	C7H12	10
19.	1,2-Diheptylcyclopropene	236	C17H32	9
20.	Ethanone, 1-(1-methyl-2-cyclopenten-1-yl	124	C8H12O	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	40	007683-64-9	99537	58	97	2	99	32	16	15	37	8274
2.	40	000000-00-0	99541	56	101	1	88	32	16	12	34	8201
3.	37	007683-64-9	136174	45	115	2	95	41	13	0	37	6664
4.	32	074793-59-2	60565	42	92	2	95	49	9	7	34	7590
5.	32	004602-84-0	129877	45	82	2	85	50	9	4	35	7366
6.	25	000142-50-7	129865	44	87	3	99	54	7	0	35	7324
7.	25	022489-66-3	60425	49	113	3	99	53	7	0	31	7286
8.	25	007212-44-4	44951	44	93	2	99	54	7	0	35	6970
9.	25	000000-00-0	44952	44	87	3	99	54	7	0	35	7324
10.	22	004602-84-0	129871	43	93	0	68	64	5	14	41	6667
11.	16	041702-60-7	11999	53	53	1	79	57	3	5	32	6743
12.	16	000142-50-7	129864	47	99	1	74	57	3	0	34	7063
13.	12	056292-64-9	32164	52	70	2	75	64	2	1	35	5798
14.	12	018794-84-8	36642	49	74	2	98	64	2	0	31	6769
15.	*10	031969-27-4	24598	35	56	1	78	76	1	0	39	5854
16.	*10	055956-43-9	4149	38	46	2	76	74	1	9	38	6138
17.	*10	041158-41-2	643	40	57	2	82	73	1	0	39	6054
18.	*10	000591-47-9	117617	42	40	0	64	76	1	11	38	5710
19.	9	035365-53-8	51031	43	93	2	66	72	1	0	34	6416
20.	* 9	068752-16-9	4791	28	51	2	95	74	1	0	33	6143

Peak 82



Average of 30.418 to 30.451 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	227	68.00	40	82.95	333	93.85	86
48.80	14	69.00	397	83.65	23	95.90	32
50.90	107	69.90	38	83.90	82	96.95	7
54.90	282	72.95	27	84.95	217	102.95	42
55.95	207	73.30	18	85.75	28	107.00	27
57.95	78	74.80	31	86.00	23	108.95	45
58.80	81	75.80	47	86.95	43	110.00	71
60.75	22	76.00	39	88.90	25	110.25	25
63.75	19	76.90	180	90.95	198	112.85	54
66.00	42	77.80	75	91.90	28	114.95	232
66.95	59	78.95	74	92.95	13	115.95	60

Average of 30.418 to 30.451 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.95	136	132.00	34	157.00	118	173.05	398
117.90	28	132.90	200	159.00	510	174.10	94
118.90	124	139.00	22	159.90	25	176.05	27
121.95	31	140.95	238	160.90	16	177.00	44
122.95	44	141.90	28	162.75	25	177.95	27
123.85	48	142.95	98	164.90	117	179.00	68
124.95	43	146.95	148	165.95	35	180.05	17
126.95	72	149.00	10	167.15	22	185.05	280
127.95	112	151.95	31	168.90	49	185.75	22
128.95	184	152.90	120	171.00	174	186.00	46
130.95	119	154.95	109	172.20	15	187.90	15

Average of 30.418 to 30.451 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
189.90	14	240.75	12				
190.90	26	242.00	11				
192.25	15	251.95	13				
193.15	23	255.20	434				
197.05	19	256.05	97				
199.00	70	270.15	92				
203.95	16						
210.90	13						
213.00	74						
235.90	17						
237.00	121						

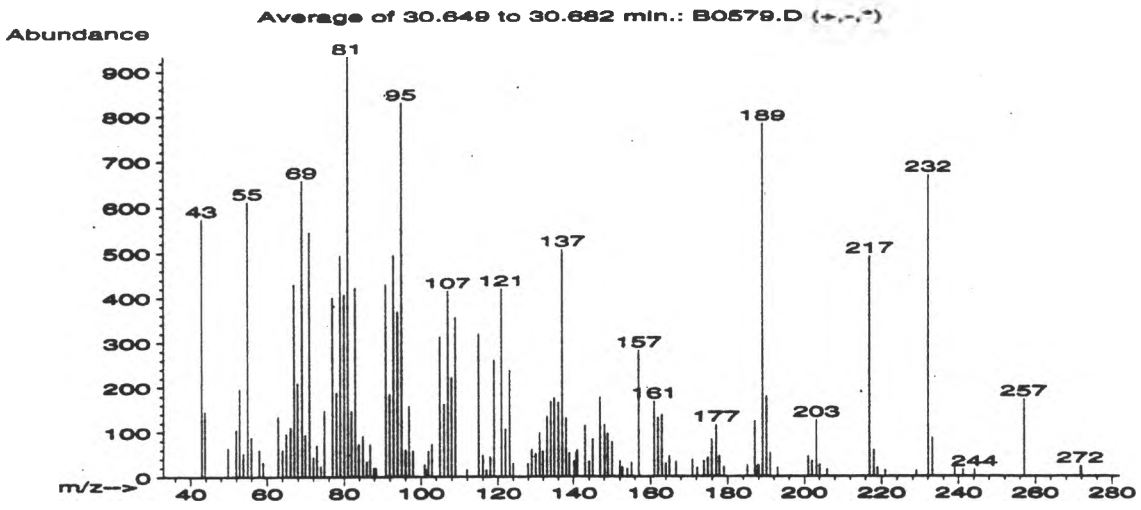
Average of 30.418 to 30.451 min.: B0579.D
Converted from RTE data file: >B0579:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3-METHOXY-4'-NITROSTILBENE	255	C15H13NO3	10
2.	Celorbicol	270	C15H26O4	9
3.	Spiro[azetidine-2,9'-fluoren]-4-one, 3-e	401	C29H23NO	9
4.	Benzamide, 2,6-dichloro-	189	C7H5Cl2NO	9
5.	1-Dicyanomethylene-cis-2,5-dimethylcyclo	174	C11H14N2	9
6.	.alpha.-D-Galactopyranoside, methyl 2-(a	393	C16H35NO6Si2	9
7.	Propanedioic acid, dibutyl-, diethyl est	272	C15H28O4	9
8.	3-Imidazoline(1-N)-3-oxide-1-oxyl, 2,2,4	171	C8H15N2O2	9
9.	Disiloxane, 1-ethenyl-1,1,3,3-tetramethy	200	C9H20OSi2	9
10.	2-Butenedioic acid, 2-methoxy-, dimethyl	174	C7H10O5	9
11.	Cyclohexanone, 4-methyl-, O-methyloxime	141	C8H15NO	9
12.	1-Fluoromethyl-4-methylnaphthalene	174	C12H11F	8
13.	(5R)-5-Iodomethyl-2,2,4,4,-tetramethyl-1	270	C8H15IO2	7
14.	4-NITRO-4'-METHOXYSTILBENE	255	C15H13NO3	7
15.	6-Deoxy-1,2-O-isopropylidene-3-O-methyl-	241	C11H15NO5	7
16.	1H-1,5-Benzodiazepine, 2,3-dihydro-2,2,4	188	C12H16N2	7
17.	9-ARISTOLEN-1.ALPHA.-OL	220	C15H24O	7
18.	3-METHOXY-4,4,4-TRIFLUORO-2-BUTENOIC ACI	170	C5H5F3O3	7
19.	1-(1,2,2-TRIMETHYLCYCLOPENT-1-YL)-PENTAN	210	C13H22O2	7
20.	2,2-DICHLORO-4,6-BIS(TRIFLUOROMETHYL)-1-	288	C4HBCl2F6N2O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*10	000000-00-0	58518	37	69	0	58	77	1	4	39	4327
2.	* 9	059812-41-8	63508	38	110	3	149	74	1	1	36	7218
3.	9	015183-53-6	136053	39	75	0	85	79	1	0	33	4327
4.	9	002008-58-4	29472	44	79	2	78	79	1	0	35	3968
5.	* 9	000000-00-0	23120	35	82	2	100	80	1	0	35	5884
6.	9	056196-93-1	96628	48	125	3	78	80	1	0	31	4651
7.	9	000596-75-8	64217	41	97	0	55	78	1	0	33	4208
8.	* 9	072960-74-8	21798	39	83	2	98	74	1	0	33	4818
9.	9	055967-53-8	34540	43	84	2	99	74	1	0	34	5684
10.	* 9	026579-97-5	126285	40	91	2	59	80	1	10	30	5252
11.	* 9	039477-43-5	9696	48	70	1	62	76	1	0	33	4591
12.	* 8	079797-78-7	23147	31	36	2	124	69	1	0	27	6683
13.	7	086547-32-2	63245	37	74	2	85	73	1	0	21	5223
14.	* 7	000000-00-0	58519	31	49	1	85	77	1	2	29	4327
15.	7	000000-00-0	52882	34	70	2	72	76	1	0	22	4518
16.	7	024107-34-4	29323	33	100	2	69	76	1	0	21	4436
17.	7	034143-95-8	44041	35	136	3	79	80	1	0	22	5423
18.	7	000000-00-0	21047	36	68	1	58	76	1	1	23	4605
19.	7	000000-00-0	39495	37	88	1	77	76	1	0	22	4574
20.	7	070613-03-5	69641	34	134	3	56	80	1	0	22	4123

Peak 107



Average of 30.649 to 30.682 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	574	62.90	135	73.95	24	86.00	33
43.75	145	63.95	60	74.85	148	86.90	72
49.80	65	64.95	96	76.95	400	87.90	20
50.85	2	66.05	110	77.95	187	88.40	20
51.90	105	67.00	430	78.95	494	90.95	429
52.85	197	67.95	209	80.00	407	91.95	184
53.90	52	69.00	657	80.95	934	92.95	494
54.95	611	69.90	94	81.95	146	94.00	367
56.00	88	70.95	546	82.95	421	94.95	829
57.95	60	71.95	44	83.85	73	95.95	60
59.00	32	72.90	71	84.95	91	96.90	157

Average of 30.649 to 30.682 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
97.90	58	114.95	318	128.95	61	140.20	34
100.95	26	116.00	48	130.00	51	140.70	54
101.70	17	116.95	15	131.00	98	140.95	59
101.95	57	118.00	44	131.90	57	143.00	114
102.90	72	119.00	260	132.95	134	144.00	33
104.95	312	119.90	1	134.00	168	144.90	84
106.00	162	120.95	420	134.95	176	146.90	177
107.00	415	121.90	106	136.00	166	148.05	116
107.95	221	123.00	238	137.00	506	148.90	97
108.95	354	123.95	30	138.00	131	150.00	77
111.90	16	127.90	29	138.90	53	152.00	34

Average of 30.649 to 30.682 min.: B0579.D
Converted from RTE data file: >B0579:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
152.30	20	170.95	37	188.00	25	218.10	59
152.70	21	172.20	20	189.00	782	219.00	20
153.95	18	173.95	34	190.00	179	220.95	14
155.05	31	174.90	42	191.00	52	228.95	13
156.95	282	175.95	83	193.00	20	232.05	667
160.95	168	177.00	115	201.00	45	233.15	86
161.95	131	177.85	45	201.95	34	239.00	21
163.00	138	179.05	21	203.15	126	241.15	15
164.00	28	185.00	24	204.05	26	244.15	15
165.00	45	187.00	123	206.05	15	257.05	172
166.75	33	187.75	25	217.00	490	271.70	23

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
271.95	22						

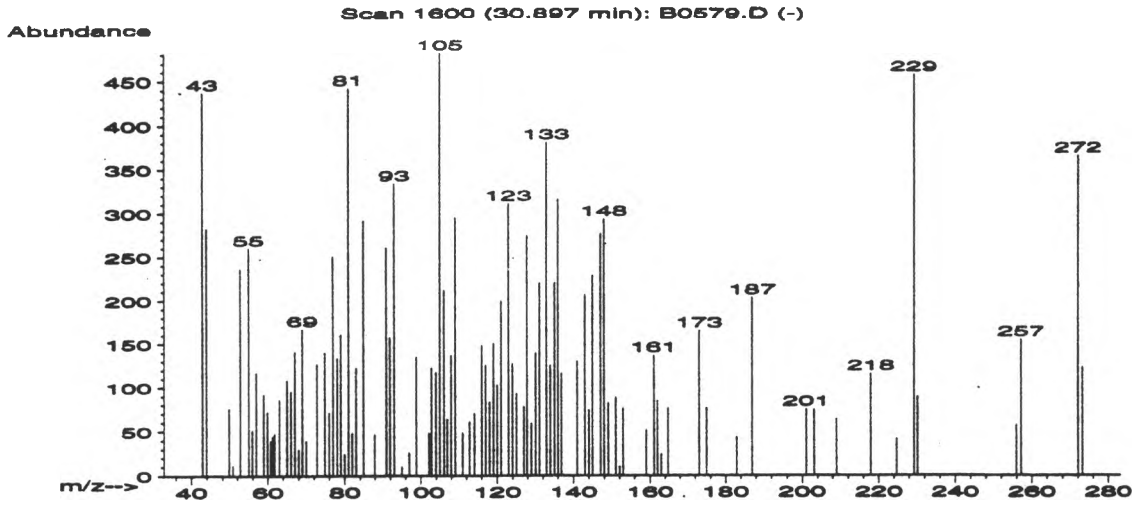
Average of 30.649 to 30.682 min.: B0579.D
Converted from RTE data file: >B0579:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	ISOCRITONILIDE	232	C15H20O2	83
2.	1-TERT-BUTYL-1,5-CYCLOOCTADIENE	164	C12H20	70
3.	Costunolide	232	C15H20O2	50
4.	Costunolide	232	C15H20O2	35
5.	1H-Indene, 1-(1,5-dimethyl-2-hexenyl)oct	248	C18H32	27
6.	1H-Pyrrole, 1-pentyl-	137	C9H15N	25
7.	Furan, 2-[(2-ethoxy-3,4-dimethyl-2-cyclo	232	C15H20O2	22
8.	2-Cyclohexylmethylenecyclopropane	136	C10H16	22
9.	11H-INDENO(1,2-B)QUINOXALIN-11-ONE	232	C15H8N2O	14
10.	4-METHYL-4-TERT-BUTYL-1-PHENYLTHIO-1-CYC	232	C15H20S	11
11.	2-Propanone, 1-(1-cyclohexen-1-yl)-	138	C9H14O	11
12.	6,6-Dimethylcycloocta-2,4-dien-1-one	150	C10H14O	11
13.	(3-(3A.ALPHA.,4A.ALPHA.,5.ALPHA.,9A.BETA	232	C15H20O2	11
14.	1H-Pyrrole, 1-butyl-	123	C8H13N	10
15.	1-Cyclohexene-1-acetonitrile	121	C8H11N	10
16.	2-Cyclopentene-1-carboxylic acid, 3,4-di	154	C9H14O2	10
17.	Bicyclo[2.2.1]heptane-2-carboxaldehyde,	124	C8H12O	10
18.	3-METHYL-7-CHLORO-2H,3H-1,2,4-BENZOTHIAD	232	C8H9ClN2O2S	10
19.	Copper chelate of 2-Nitroso-4-methylguai	167	C8H9NO3	10
20.	5-Methylene-cis-hydrindan-2-one	150	C10H14O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	062458-57-5	49264	31	14	0	48	0	50	1	42	.4387
2.	*70	000000-00-0	18734	94	33	1	77	65	41	0	93	5514
3.	*50	000553-21-9	130442	63	114	3	99	48	25	0	64	7397
4.	*35	000553-21-9	49243	70	99	2	97	51	11	0	41	8239
5.	27	054411-95-9	55830	74	81	3	89	58	8	0	40	7080
6.	*25	000699-22-9	8321	33	67	0	71	63	7	16	43	6530
7.	*22	055162-49-7	49232	66	93	2	67	63	5	0	39	7060
8.	22	057497-09-3	8141	59	46	0	97	63	5	0	43	5995
9.	*14	006954-91-2	49207	33	31	0	51	70	2	0	41	3544
10.	*11	000000-00-0	49280	34	43	0	48	80	2	4	43	5297
11.	*11	000768-50-3	8638	55	57	1	72	73	2	0	49	5055
12.	*11	091531-51-0	12795	51	70	1	51	77	2	0	44	5052
13.	*11	066873-37-8	49267	52	86	1	53	78	2	0	44	6154
14.	*10	000589-33-3	4591	36	56	0	72	74	1	0	41	5508
15.	*10	006975-71-9	4257	37	59	0	83	75	1	6	39	5357
16.	*10	062185-63-1	14405	36	54	2	88	74	1	18	40	4871
17.	*10	003574-55-8	4822	36	55	0	76	80	1	0	41	4882
18.	*10	022503-72-6	48873	40	105	0	54	75	1	0	39	4351
19.	*10	000000-00-0	19861	46	47	1	50	80	1	0	39	3078
20.	*10	092464-23-8	12824	53	49	0	52	76	1	1	40	6939

Peak 83



Scan 1600 (30.897 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	437	61.25	44	75.95	71	91.95	157
43.90	282	61.75	47	76.95	250	93.00	333
49.80	76	63.00	86	78.05	134	94.95	10
50.80	11	64.95	108	78.95	161	96.95	26
52.80	236	66.00	95	79.95	24	98.80	135
54.95	260	67.00	141	80.95	442	102.05	48
55.90	51	68.00	30	81.95	48	102.80	122
56.90	117	68.95	167	82.90	122	103.95	117
58.90	92	69.95	39	84.90	291	104.95	481
59.90	72	72.80	127	87.90	46	106.05	211
60.75	39	74.80	140	91.00	260	106.95	64

Scan 1600 (30.897 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
107.90	137	122.95	310	136.00	315	152.95	76
109.00	294	123.95	127	136.90	116	159.00	51
110.95	48	124.95	93	141.00	130	161.00	137
112.75	61	126.95	78	143.00	206	162.00	85
114.00	70	127.80	273	144.00	74	162.95	24
116.00	148	128.95	59	144.95	228	164.75	76
117.00	125	130.05	139	146.95	276	173.05	165
118.00	83	131.05	219	147.95	293	175.05	76
119.00	150	132.90	380	149.00	82	182.90	43
119.95	102	133.90	125	150.95	88	187.00	203
120.95	199	135.00	220	151.95	10	201.05	75

Scan 1600 (30.897 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
203.05	74						
209.00	64						
218.00	116						
224.70	41						
229.20	457						
230.20	89						
255.95	57						
257.20	155						
272.05	365						
273.20	123						

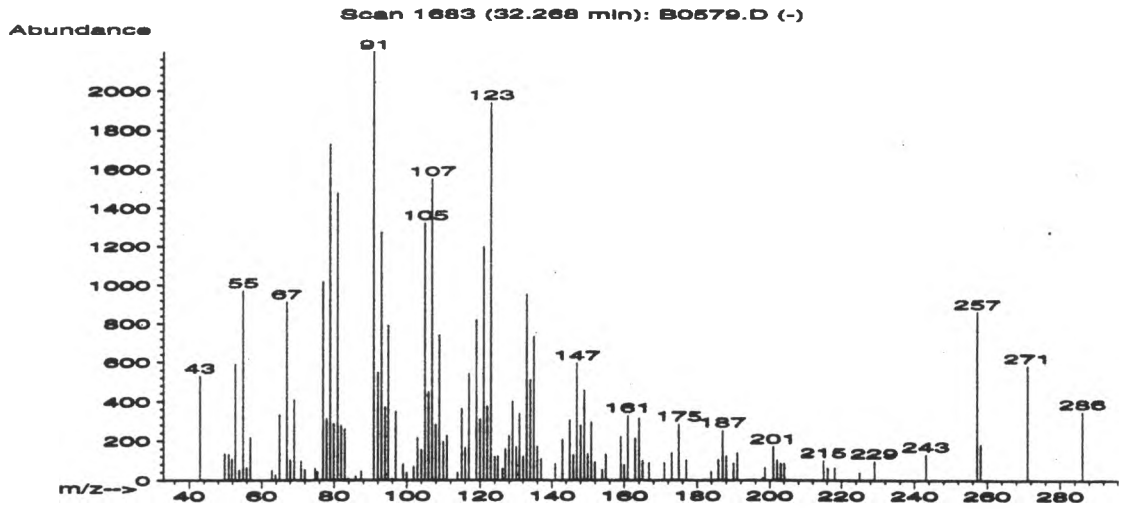
Scan 1600 (30.897 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1H-Pyrrole, 1-(2-furanylmethyl)-	147	C9H9NO	14
2.	N-FURFURYL PYRROLE	147	C9H9NO	14
3.	2(S),3(S)-(Isopropylidenedioxy)-4(R)-(Z)	196	C11H16O3	12
4.	2-Cyclopenten-1-one, 2,3,5-trimethyl-4-m	136	C9H12O	11
5.	12-O-METHYLPODOCARPINAL	272	C18H24O2	11
6.	Phenol, 2-methyl-6-(2-propenyl)-	148	C10H12O	10
7.	2,5-DIMETHYL-3-TRANS-PROPENYLPYRAZINE	148	C9H12N2	10
8.	N,N-DIETHYL-2,4-PENTADIENEOIC ACID AMIDE	153	C9H15NO	10
9.	Isopimaradiene	272	C20H32	10
10.	6-METHYL-4,5-DIPHENYL-4H-CYCLOPENTA[B]FU	272	C20H16O	10
11.	TRANS-10-PHENYL-2-DECALONE-9-D	228	C16H19DO	10
12.	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	10
13.	ANTI,SYN,ANTI-3,3,6,6,9,9,12,12-OCTAMETH	272	C20H32	10
14.	1-AZACHRYSENE	229	C17H11N	10
15.	s-Triazolo[4,3-a]pyridine, 3-amino-6-met	148	C7H8N4	10
16.	3,6-ISO BENZOFUROQUINONE	148	C8H4O3	10
17.	2,5-Heptadiene, (E,E)-	96	C7H12	10
18.	s-Triazolo[4,3-a]pyridine, 3-amino-5-met	148	C7H8N4	10
19.	1,3-DIMETHYL-3,4-DIHYDRO-PYRROLO(1,2-A)P	148	C9H12N2	10
20.	1,4-DIMETHYL-3,4-DIHYDRO-PYRROLO(1,2-A)P	148	C9H12N2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*14	001438-94-4	11657	33	56	1	91	68	2	0	41	4267
2.	*14	000000-00-0	11656	33	40	1	91	68	2	0	39	4252
3.	12	077761-77-4	32865	46	118	2	86	63	2	0	35	2806
4.	*11	029765-85-3	7890	50	60	1	144	75	2	0	44	2604
5.	*11	016826-83-8	64355	43	114	0	62	77	2	0	44	6510
6.	*10	003354-58-3	12092	35	85	0	60	80	1	0	41	5579
7.	*10	000000-00-0	11975	35	76	1	76	75	1	0	39	6108
8.	*10	000000-00-0	14066	39	62	0	72	75	1	0	39	2604
9.	10	001686-66-4	132293	60	133	3	121	74	1	0	39	7082
10.	*10	086738-92-3	64430	35	114	0	75	73	1	6	39	5036
11.	*10	027863-66-7	47836	34	53	0	85	80	1	4	39	5041
12.	*10	000122-03-2	123388	36	79	0	78	80	1	0	41	5597
13.	*10	000000-00-0	64473	76	115	2	75	72	1	13	38	6629
14.	*10	000000-00-0	48070	39	90	0	95	80	1	0	39	5041
15.	*10	005528-60-9	11878	34	85	0	59	80	1	0	41	3842
16.	*10	000000-00-0	11913	35	74	1	60	80	1	0	39	3792
17.	10	039619-60-8	614	47	54	1	91	75	1	1	38	2720
18.	*10	005595-15-3	11877	33	77	0	46	80	1	0	41	3943
19.	*10	064608-67-9	11988	37	66	0	73	80	1	0	41	5763
20.	*10	064608-68-0	11989	40	76	0	60	78	1	0	39	5944

Peak 86



Scan 1683 (32.268 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	529	65.00	334	78.95	1727	93.00	1276
49.80	134	67.00	912	79.95	288	94.00	371
50.95	133	68.00	101	80.95	1478	94.90	790
51.80	109	69.00	408	81.95	279	95.95	8
52.80	590	70.00	3	82.90	261	96.95	349
53.90	52	70.90	96	83.95	8	98.95	81
54.95	972	71.95	53	85.90	20	99.95	38
55.95	66	74.80	60	87.40	47	101.80	69
56.95	218	75.45	44	87.70	5	102.90	216
62.90	51	76.95	1019	90.90	2198	103.95	155
63.85	29	77.95	312	92.00	547	104.95	1320

Scan 1683 (32.268 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
105.95	447	120.05	310	130.95	338	146.95	596
106.95	1546	120.95	1196	132.05	121	147.95	281
107.90	283	121.95	373	133.00	950	148.95	457
108.90	741	122.95	1934	134.00	510	149.95	135
109.90	195	124.00	120	135.00	732	150.95	297
110.90	228	124.95	123	136.00	171	151.95	91
113.90	40	126.20	60	137.00	109	153.95	54
115.00	362	126.95	160	140.95	83	154.95	131
116.00	166	127.95	228	143.00	207	159.00	222
117.00	542	128.95	403	144.95	306	160.00	78
119.00	819	129.95	170	145.95	129	161.00	329

Scan 1683 (32.268 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
163.00	212	188.00	123	218.15	64		
164.00	316	190.00	86	224.95	40		
165.00	101	191.00	140	229.05	99		
166.75	88	198.00	13	243.15	131		
170.90	89	198.70	66	257.20	861		
172.95	139	201.05	172	258.15	180		
174.95	285	202.05	104	271.05	580		
176.95	103	203.05	85	286.15	349		
183.90	46	204.05	87				
185.90	105	215.00	101				
187.00	255	216.15	64				

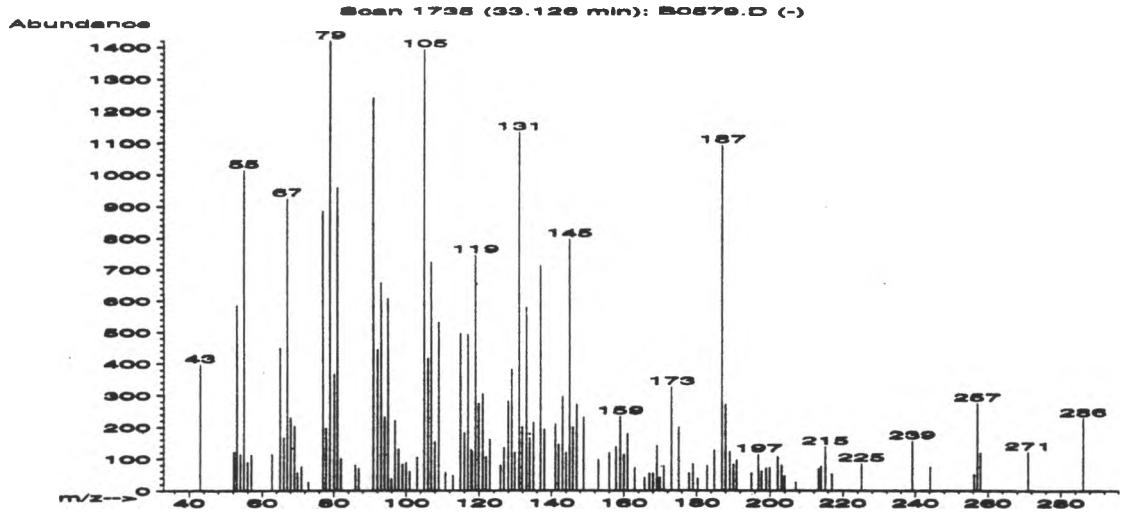
Scan 1683 (32.268 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	SPIRO[2.9]DODECA-3,7-DIENE, 11,11-DIMETH	190	C14H22	49
2.	TRICYCLO[3.1.0.0(2,4)]HEXANE, 3,6-DIETHY	164	C12H20	42
3.	TRICYCLO[3.2.1.0(2,8)]OCTAN-7-ONE, 6-MET	190	C13H18O	30
4.	1,5-Hexadiene, 2,5-dimethyl-3-methylene-	122	C9H14	20
5.	Benzenemethanol, .alpha.-methyl-	122	C8H10O	20
6.	Benzenemethanol, .alpha.-methyl-	122	C8H10O	18
7.	Benzenemethanol, .alpha.-methyl-	122	C8H10O	18
8.	Cyclohexane, 1,5-diethenyl-2,3-dimethyl-	164	C12H20	18
9.	CYCLOHEXANE,2A,3E-DIMETHYL-1E,5A-DIVINYL	164	C12H20	18
10.	.alpha.-Sinensal	218	C15H22O	14
11.	6,6-Dimethylcycloocta-2,4-dien-1-one	150	C10H14O	14
12.	trans-Caryophyllene	204	C15H24	14
13.	.BETA.-D3-1-PHENYLETHANOL-1	122	C8H7D3O	14
14.	Benzenemethanol, .alpha.-(aminomethyl)-	137	C8H11NO	14
15.	exo-4-Methylbicyclo[3.2.1]octan-3-ene	122	C9H14	11
16.	1,3,6-Octatriene, (Z,E)-	108	C8H12	11
17.	Benzenemethanol, 3-amino-	123	C7H9NO	11
18.	POLYUNSATURATED FATTY ACID METHYL ESTER	342	C23H34O2	10
19.	2,6-DIMETHYL-4-PYRIDINOL	123	C7H9NO	10
20.	Phenol, 2-amino-5-methyl-	123	C7H9NO	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	000000-00-0	30227	86	66	1	53	62	23	0	87	6888
2.	*42	078578-91-3	18768	75	40	0	63	60	17	41	74	6025
3.	*30	000000-00-0	30176	68	81	2	75	56	9	29	47	7416
4.	*20	059131-13-4	4462	68	43	0	73	67	4	25	58	6604
5.	*20	000098-85-1	120231	68	33	0	59	66	4	41	58	6728
6.	*18	000098-85-1	120229	48	55	1	70	66	3	0	46	6587
7.	*18	000098-85-1	120232	44	58	0	56	66	3	0	44	6695
8.	*18	068779-14-6	18729	60	70	2	70	70	3	0	46	6839
9.	*18	068779-12-4	18731	60	70	2	70	70	3	0	46	6839
10.	*14	017909-77-2	129600	45	103	3	129	67	2	0	39	6596
11.	14	091531-51-0	12795	61	65	2	77	66	2	0	39	6753
12.	*14	000087-44-5	128689	76	66	1	71	70	2	18	40	6545
13.	14	017537-32-5	4400	45	46	0	55	67	2	19	41	6469
14.	*14	007568-93-6	8309	34	57	2	430	67	2	0	41	6599
15.	*11	078965-86-3	4484	47	49	0	65	77	2	0	44	5440
16.	*11	022038-68-2	1939	52	55	0	55	78	2	0	46	4921
17.	*11	001877-77-6	4580	49	58	2	81	77	2	24	47	5659
18.	10	000000-00-0	86199	62	77	0	60	78	1	0	43	4921
19.	*10	000000-00-0	4565	33	51	1	65	78	1	0	41	5511
20.	*10	002835-98-5	4587	45	56	1	60	77	1	0	39	5588

Peak 108



Scan 1735 (33.126 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	396	68.00	230	85.90	80	99.95	88
52.20	122	69.00	203	86.90	70	100.95	60
52.95	585	69.95	56	90.90	1241	102.95	106
54.00	115	70.95	76	92.00	443	104.95	1392
54.95	1015	72.95	27	93.00	655	106.05	416
55.95	90	76.95	886	93.95	231	106.95	723
57.00	113	77.85	197	94.95	605	107.90	155
62.75	116	78.95	1421	95.95	37	109.00	530
64.90	449	80.05	367	96.95	220	110.85	58
66.00	167	80.95	959	97.95	130	112.90	47
67.00	925	81.95	100	98.95	83	114.90	495

Scan 1735 (33.126 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
116.00	182	127.95	283	141.90	146	160.00	115
117.00	491	128.95	382	143.00	296	161.00	180
117.90	129	129.80	121	144.00	120	163.00	72
118.15	124	131.05	1130	144.95	795	165.65	41
119.00	745	131.90	202	145.95	201	167.00	54
119.95	273	133.00	578	147.05	270	168.00	54
120.95	305	133.90	166	148.95	231	169.00	141
121.85	108	135.00	214	152.95	98	169.80	42
122.95	162	136.95	712	156.05	120	170.90	78
125.80	81	138.00	193	157.90	138	173.05	326
126.80	136	141.00	209	159.00	233	175.05	200

Scan 1735 (33.126 min): B0579.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
177.95	54	196.95	115	217.00	52		
179.05	84	197.80	61	225.05	86		
180.30	38	198.95	71	239.15	157		
182.95	78	199.95	73	244.15	75		
184.90	127	202.05	108	256.20	50		
187.00	1090	203.20	80	257.05	274		
188.00	271	203.95	46	258.00	120		
189.15	123	207.00	28	271.05	122		
190.15	83	213.25	69	286.15	228		
191.00	96	213.90	77				
195.05	56	215.15	138				

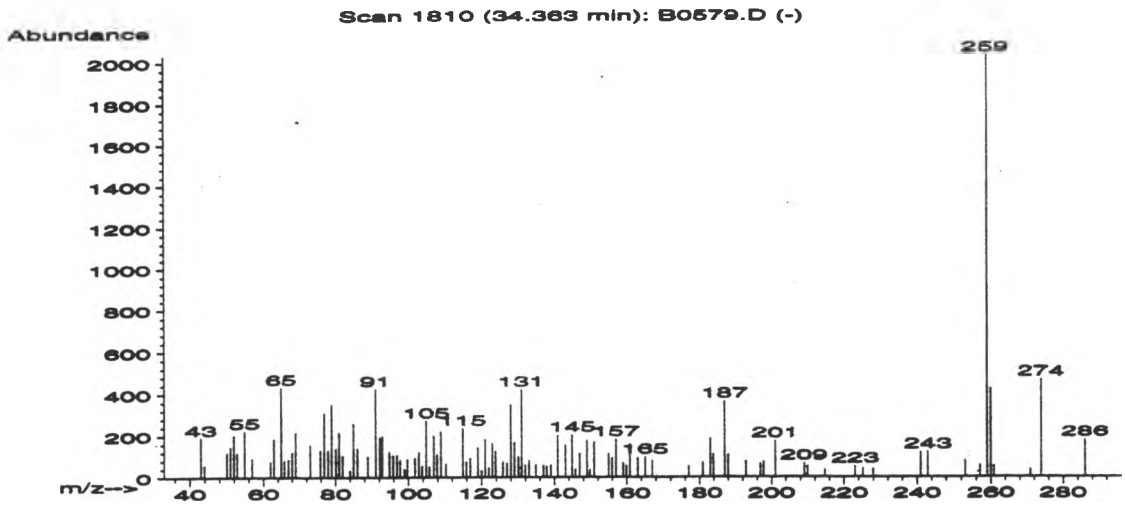
Scan 1735 (33.126 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclopentaneacetaldehyde, 2-formyl-3-met	166	C10H14O2	38
2.	trans-Caryophyllene	204	C15H24	27
3.	Patchoulane	206	C15H26	22
4.	Methyl 2,3-dimethyl-5-(3'-methyl-2'H-pyr	250	C15H22O3	22
5.	3,3-DICHLORO-1,1,2,2-TETRAMETHYL-CYCLOPR	166	C7H12Cl2	22
6.	METHYL 12-VINYLCYCLODODECA-1,4,8-TRIENEC	246	C16H22O2	16
7.	(E)-AND(Z)-7-METHYL-5,7-OCTADIEN-1-OL	140	C9H16O	12
8.	1-(1,3-BUTADIENE-2-YL)-CYCLOPENTANOL	138	C9H14O	12
9.	Patchulane	206	C15H26	12
10.	3-Methylene-1,6-hexadiene	108	C8H12	11
11.	1,4-Methanonaphthalen-9-ol, 1,2,3,4-tetr	160	C11H12O	10
12.	4-,,inside''-Methyl-endo,exo-tetracyclo[	192	C13H20O	10
13.	3,4-DIMETHYL-5-(3-METHYLPHENYL)ISOXAZOLE	187	C12H13NO	10
14.	3,4-DIMETHYL-5-(4-METHYLPHENYL)ISOXAZOLE	187	C12H13NO	10
15.	CIS/TRANS-7-BICYCLO[4.1.0]HEPT-7-YLIDENE	188	C14H20	10
16.	Benzene, 1-(5,5-dimethyl-1-cyclopenten-1	202	C14H18O	10
17.	12-Oxapentacyclo[7.2.1.0(2,7).0(2,8).0(3	160	C11H12O	10
18.	2-METHYL-2H-NAPHTHO(1,8-B,C)THIOPHEN-3-O	202	C12H10OS	10
19.	2-Amino-1,4-dimethyl-5-phenylimidazole h	187	C11H13N3	10
20.	Mixture of trans,trans-1,3-Dimethylenecy	188	C14H20	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*38	005951-57-5	19396	68	63	1	89	63	14	0	68	4248
2.	27	000087-44-5	128695	71	71	2	140	56	8	0	38	5576
3.	22	025491-20-7	37750	61	84	0	52	64	5	0	43	4967
4.	22	088354-67-0	56494	58	120	3	106	63	5	0	39	5263
5.	22	000000-00-0	19172	45	62	2	124	65	5	11	38	6151
6.	16	057709-14-5	54903	54	71	1	102	58	3	10	37	7823
7.	12	064275-81-6	9361	46	54	1	95	65	2	0	37	3836
8.	12	000000-00-0	8613	55	80	2	57	65	2	0	36	3486
9.	12	019078-35-4	37751	44	87	1	104	61	2	0	37	4694
10.	*11	016626-48-5	1950	48	64	3	152	71	2	0	44	3166
11.	*10	013999-10-5	16977	38	58	0	54	80	1	0	39	4728
12.	10	080183-77-3	31079	44	85	1	61	80	1	11	38	5479
13.	*10	061314-42-9	28853	38	77	0	63	78	1	0	39	5492
14.	*10	061314-43-0	28854	56	67	1	70	75	1	0	40	5812
15.	*10	000000-00-0	29441	59	87	2	147	74	1	0	39	6602
16.	10	039877-93-5	35706	47	96	1	70	67	1	0	35	6789
17.	*10	071794-80-4	16986	40	17	0	62	80	1	5	38	4728
18.	*10	067260-08-6	35551	37	70	1	59	75	1	18	40	4636
19.	*10	058325-33-0	28836	36	28	0	64	71	1	0	41	5461
20.	*10	066405-18-3	29413	43	47	0	74	71	1	0	39	6505

Peak 109



Scan 1810 (34.363 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.95	191	65.85	81	80.95	217	96.95	108
43.90	60	66.95	87	81.95	105	97.80	85
49.95	121	68.00	122	84.00	35	98.95	40
50.95	147	68.95	216	85.00	260	99.80	86
51.95	203	69.95	2	86.00	139	101.80	93
52.80	119	72.95	157	88.90	101	102.85	122
54.90	224	75.80	130	91.00	425	103.80	55
56.95	90	76.90	309	92.15	192	104.95	272
61.90	76	77.95	130	92.90	198	105.85	52
62.90	186	78.95	350	94.90	124	107.00	200
64.90	433	80.05	140	95.80	106	107.90	109

Scan 1810 (34.363 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
108.95	221	125.80	75	139.00	59	157.05	183
110.25	65	126.95	69	140.90	202	158.95	69
114.90	236	127.95	348	143.00	155	159.90	55
115.90	76	128.95	169	144.95	204	160.90	129
116.95	92	130.05	98	145.80	38	163.00	94
119.00	146	130.90	422	146.95	114	165.00	99
119.95	33	131.90	60	149.00	179	167.00	79
120.95	181	133.00	81	149.85	36	176.95	53
121.95	45	134.95	61	150.95	171	180.90	69
122.95	165	137.00	58	154.95	115	183.00	186
123.80	127	137.90	52	155.95	93	183.90	109

Scan 1810 (34.363 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
187.00	364	223.05	54	273.95	465		
188.00	108	225.20	42	286.00	178		
192.90	77	227.95	38				
196.95	64	241.00	121				
197.80	76	243.00	122				
201.05	174	253.05	78				
206.95	2	256.95	57				
208.80	3	259.00	2034				
209.00	67	260.00	421				
209.90	54	260.90	53				
214.75	36	270.95	36				

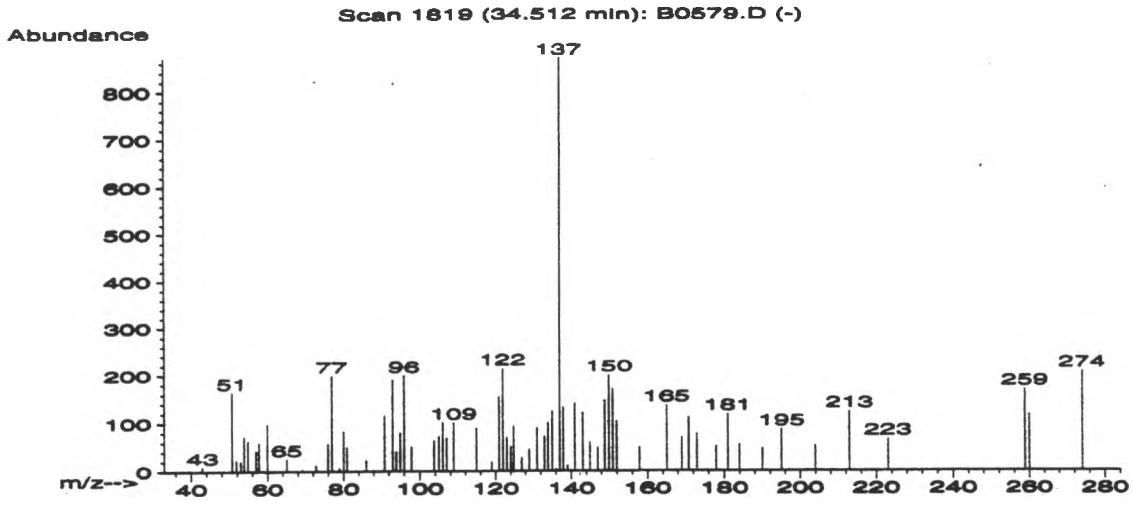
Scan 1810 (34.363 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benz[c]acridin-7(12H)-one, 11-methyl-	259	C18H13NO	46
2.	2,6 Di-p-tolylpyridine	259	C19H17N	43
3.	Benzenamine, 2,4-dinitro-N-phenyl-	259	C12H9N3O4	43
4.	Benz[a]anthracen-7(12H)-one, 12-hydroxy-	274	C19H14O2	40
5.	1H-Indene-4-acetic acid, 6-(1,1-dimethyl	274	C18H26O2	38
6.	Furo[2,3-b]quinoline, 4,6,7-trimethoxy-	259	C14H13NO4	38
7.	HAPTO-5-PENTAMETHYLCYCLOPENTADIENYL-HAPT	259	C15H20Co	38
8.	Silane, methyltriphenyl-	274	C19H18Si	37
9.	Benzenamine, 4-nitro-N-(4-nitrophenyl)-	259	C12H9N3O4	37
10.	Furo[2,3-b]quinolin-4(9H)-one, 7,8-dimet	259	C14H13NO4	37
11.	[2](1,5)NAPHTHALINO[2](2,6)PYRIDINOPHANE	259	C19H17N	37
12.	Benzenamine, 2-nitro-N-(2-nitrophenyl)-	259	C12H9N3O4	32
13.	10H-Phenoxaphosphine, 2-ethyl-10-hydroxy	274	C15H15O3P	32
14.	13,13-DIMETHYLPODOCARP-7-EN-8-ONE	274	C19H30O	30
15.	Benzenamine, 2-nitro-N-(4-nitrophenyl)-	259	C12H9N3O4	28
16.	Silane, [(pentafluorophenyl)thio]triphen	458	C24H15F5SSi	25
17.	1-(1-METHYL-2-PHENETHYL)-4-(N-PROPANILID	350	C23H30N2O	25
18.	1-(2-Phenylethyl)-4-(N-propananilido)-ci	350	C23H30N2O	25
19.	[2](1,4)NAPHTHALINO[2](2,6)PYRIDINOPHANE	259	C19H17N	25
20.	Furo[2,3-b]quinoline, 4,6,8-trimethoxy-	259	C14H13NO4	23

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*46	077745-36-9	59335	53	78	1	84	44	20	0	47	9347
2.	*43	014435-88-2	59348	60	66	0	71	44	18	14	41	9347
3.	*43	000961-68-2	59199	36	104	2	94	44	18	0	39	9333
4.	*40	017513-39-2	65086	34	87	0	71	33	16	8	35	9579
5.	38	055591-15-6	65070	45	100	2	93	37	14	0	37	9564
6.	*38	000484-08-2	59242	37	112	1	99	38	14	0	30	9369
7.	*38	000000-00-0	59279	38	82	0	74	50	14	5	40	9341
8.	*37	000791-29-7	65109	34	91	2	96	44	13	1	32	9531
9.	*37	001821-27-8	59202	41	103	2	97	41	13	0	35	9359
10.	*37	000436-14-6	59240	33	82	1	99	44	13	0	35	9339
11.	*37	000000-00-0	59346	38	105	2	85	44	13	0	33	9347
12.	*32	018264-71-6	59200	35	114	2	78	48	9	0	35	9359
13.	32	036360-91-5	64928	45	95	2	66	50	9	0	35	8797
14.	*30	007715-44-8	65113	62	74	1	41	61	9	0	56	9233
15.	*28	000612-36-2	59201	29	109	2	99	40	8	0	29	9367
16.	25	022530-03-6	105482	41	112	1	80	44	7	0	28	9337
17.	25	000000-00-0	134960	39	100	3	99	44	7	0	29	9335
18.	25	000000-00-0	88130	42	117	3	99	41	7	0	28	9417
19.	*25	000000-00-0	59347	24	81	2	99	44	7	6	23	9347
20.	*23	000522-19-0	59243	29	132	2	77	47	6	0	27	9345

Peak 110



Scan 1819 (34.512 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.90	9	72.80	12	95.95	199	122.95	70
50.70	164	75.95	57	97.80	50	124.00	51
51.75	23	76.95	199	103.70	63	124.80	93
52.95	20	78.85	6	105.00	73	126.95	28
53.80	72	79.95	83	105.95	101	128.95	45
54.80	63	80.95	50	107.00	69	131.00	89
56.95	43	85.90	22	108.90	101	132.90	71
57.75	59	90.90	115	114.95	89	133.90	100
59.90	98	93.00	190	118.95	19	135.00	124
65.00	25	93.95	40	120.95	154	135.95	3
69.00	4	94.95	79	121.95	214	137.00	869

Scan 1819 (34.512 min): B0579.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.90	132	165.00	136	223.05	66		
139.00	11	169.00	69	258.85	169		
140.90	140	170.80	111	260.00	117		
143.00	121	172.95	77	274.05	207		
144.90	59	177.95	51				
146.90	48	180.95	118				
148.80	146	183.90	54				
149.95	200	189.90	46				
150.95	171	195.05	86				
151.95	104	203.95	52				
157.90	49	213.00	123				

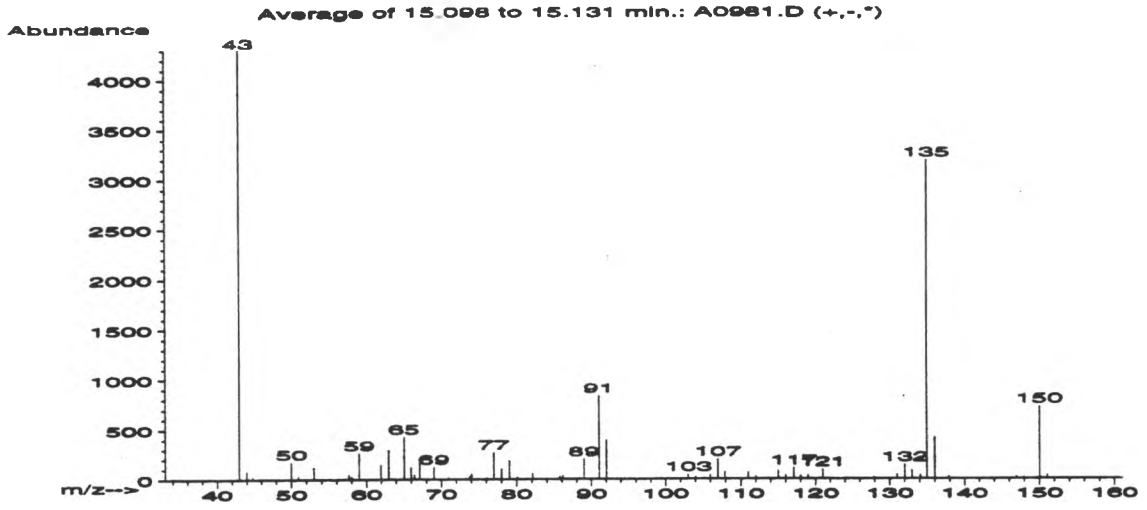
Scan 1819 (34.512 min): B0579.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	5-(ACETYLAMINOMETHYL)-4-AMINO-2-METHYLPY	180	C8H12N4O	38
2.	Copper chelate of 2-Nitroso-4-methylguai	167	C8H9NO3	37
3.	3,7-Benzofurandiol, 2,3-dihydro-2,2-dime	237	C12H15NO4	27
4.	3,6-DIMETHYL-2,3,3A,4,5,7A-HEXAHYDROBENZ	152	C10H16O	25
5.	CIS-1-TRIMETHYLSILYLHEX-3-EN-1-YNE	152	C9H16Si	25
6.	TRANS-1-TRIMETHYLSILYLHEX-3-EN-1-YNE	152	C9H16Si	22
7.	4H-1A,3,6,9,TETRAHYDROQUINOLIZINE-4,9A-D	135	C9H11D2N	22
8.	Benzaldehyde, 3-hydroxy-, oxime	137	C7H7NO2	22
9.	Benzoic acid, 4-amino-	137	C7H7NO2	22
10.	Benzoic acid, 3-amino-	137	C7H7NO2	22
11.	2,6-Pyridinedicarboxylic acid, dimethyl	195	C9H9NO4	16
12.	1-Oxaspiro[2.5]octane, 4,4-dimethyl-8-me	152	C10H16O	16
13.	4,5-DIETHYL-3-ISOPROPENYL-2,2-DIMETHYL-2	224	C11H21BSSi	12
14.	Arsenic acid (H3AsO4), triethyl ester	226	C6H15AsO4	12
15.	Benzeneacetic acid, .alpha.-hydroxy-2-me	182	C9H10O4	12
16.	4-Nitroso-3-methylphenol	137	C7H7NO2	12
17.	Benzoic acid, 3-amino-	137	C7H7NO2	12
18.	2-CYANO-1-BENZOXATHIANE	177	C9H7NOS	12
19.	2-AMINO-4,5,6,7-D4-BENZIMIDAOLE	133	C7H3D4N3	12
20.	3,5-Octadiene, 2,2,4,5,7,7-hexamethyl-,	194	C14H26	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	38	023676-63-3	25383	45	38	2	99	47	14	12	41	9049
2.	37	000000-00-0	19861	50	34	1	99	45	13	15	36	9057
3.	27	016655-82-6	51131	45	78	3	95	56	8	18	38	8756
4.	*25	070786-44-6	13847	51	46	1	82	63	7	0	46	8711
5.	*25	060216-44-6	13563	36	46	2	88	63	7	21	43	8692
6.	*22	060216-43-5	13562	41	41	1	84	63	5	16	38	8692
7.	*22	053957-27-0	7637	33	60	0	69	63	5	10	39	8767
8.	*22	022241-18-5	8270	37	38	1	76	65	5	9	38	8614
9.	*22	000150-13-0	8266	34	78	0	84	65	5	0	41	8614
10.	*22	000099-05-8	122140	36	79	1	82	65	5	0	39	8614
11.	*16	005453-67-8	32263	34	75	1	99	60	3	1	36	8646
12.	*16	054345-56-1	13767	39	82	3	71	56	3	0	35	8806
13.	12	000000-00-0	45626	38	114	2	85	60	2	0	29	8655
14.	12	015606-95-8	46357	39	84	2	67	65	2	4	31	8614
15.	12	010408-29-4	126984	52	67	3	98	63	2	0	31	8736
16.	*12	000615-01-0	8262	40	42	1	99	63	2	0	35	8751
17.	*12	000099-05-8	8265	29	74	2	74	64	2	0	33	8643
18.	12	051263-42-4	24154	44	90	1	66	63	2	0	35	8732
19.	*12	000000-00-0	7100	28	54	0	98	65	2	6	35	8614
20.	12	055712-52-2	32145	43	79	2	99	63	2	0	35	8711

Peak 111



Average of 15.098 to 15.131 min.: A0981.D
Converted from RTE data file: >A0981:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4301	65.05	428	79.05	188	106.00	39
44.00	82	66.00	120	80.05	19	107.00	197
44.80	22	66.40	42	82.10	59	107.90	69
50.00	177	67.10	182	85.75	31	111.00	65
50.95	34	69.00	123	86.15	35	112.00	24
53.00	123	70.95	15	88.40	13	115.00	83
57.65	49	73.80	32	89.00	203	116.00	37
58.00	19	74.05	54	91.05	836	117.10	111
59.00	262	76.05	13	92.05	388	118.00	32
61.95	145	77.00	270	103.05	45	119.00	36
63.00	295	78.00	106	104.05	19	121.00	96

Average of 15.098 to 15.131 min.: A0981.D
Converted from RTE data file: >A0981:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.95	16	151.05	35				
131.00	42						
132.05	143						
133.00	82						
134.10	37						
135.00	3178						
136.00	417						
137.90	23						
146.95	22						
147.95	14						
150.05	727						

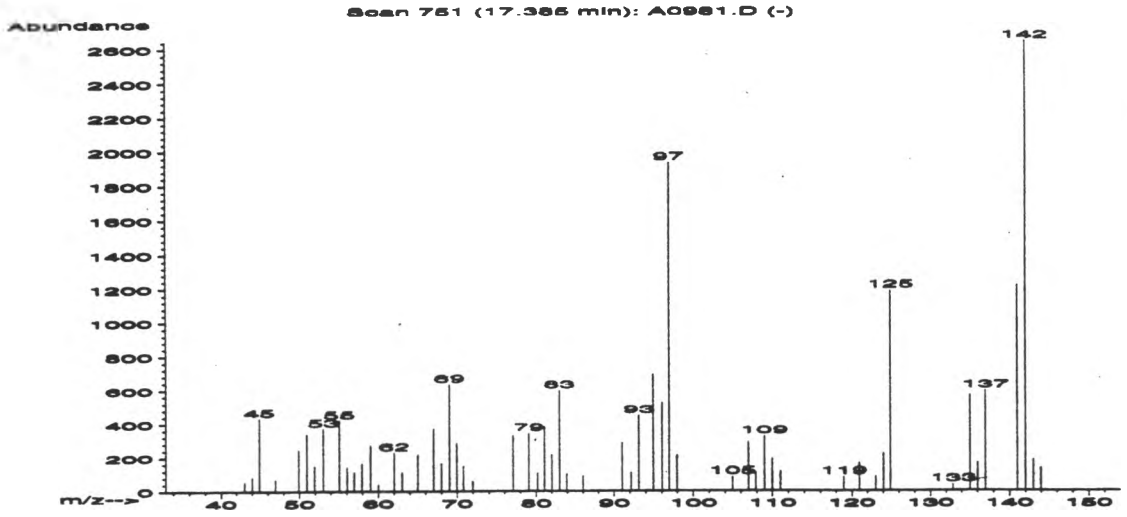
Average of 15.098 to 15.131 min.: A0981.D
Converted from RTE data file: >A0981:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Benzenemethanol, 4-(1-methylethyl)-	150	C10H14O	59
2.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	52
3.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	52
4.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	50
5.	BENZO(B)THIOPHENE-3-D	134	C8H5DS	50
6.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	50
7.	Silane, trimethylphenyl-	150	C9H14Si	49
8.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	47
9.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	47
10.	ACETOPHENONE, 2'-METHOXY-	150	C9H10O2	42
11.	Phenol, 2-(1,1-dimethylethyl)-	150	C10H14O	42
12.	Phenol, 5-methyl-2-(1-methylethyl)-	150	C10H14O	40
13.	Pyridine, 4-ethyl-2,6-dimethyl-	135	C9H13N	40
14.	1-VINYL-2,6,6-TRIMETHYLCYCLOHEX-1-ENE	150	C11H18	40
15.	Phenol, 3-(1,1-dimethylethyl)-	150	C10H14O	40
16.	Phenol, 4-(1,1-dimethylethyl)-	150	C10H14O	40
17.	Phenol, 3-methyl-5-(1-methylethyl)-, met	207	C12H17NO2	38
18.	Benzaldehyde, 4-methoxy-	136	C8H8O2	38
19.	Phenol, 2-methyl-5-(1-methylethyl)-	150	C10H14O	38
20.	Benzothiazole	135	C7H5NS	37

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	000536-60-7	12736	41	42	3	127	21	33	0	39	9794
2.	*52	000089-83-8	123678	35	52	2	68	34	27	18	43	6024
3.	*52	000098-54-4	123676	51	42	2	50	34	27	0	46	5889
4.	*50	000089-83-8	123680	38	41	2	73	35	25	10	38	6026
5.	*50	015816-45-2	7331	36	48	3	59	32	25	0	39	5880
6.	*50	000499-75-2	123688	41	50	2	50	35	25	3	38	6000
7.	*49	000768-32-1	123658	34	34	1	59	37	23	8	43	5990
8.	*47	000499-75-2	123687	45	44	2	59	37	20	0	40	6019
9.	*47	000585-34-2	123671	39	52	2	55	37	20	0	39	5908
10.	*42	000000-00-0	12617	42	50	2	64	29	17	0	35	6060
11.	*42	000088-18-6	123670	41	56	2	50	28	17	0	35	5241
12.	*40	000089-83-8	123681	44	46	2	50	35	16	1	36	6004
13.	*40	036917-36-9	7611	33	70	2	73	31	16	0	35	5935
14.	*40	005293-90-3	12922	35	68	3	67	31	16	0	35	5785
15.	40	000585-34-2	123672	45	45	2	72	34	16	17	37	5783
16.	*40	000098-54-4	123674	40	52	2	73	34	16	0	35	5870
17.	38	002631-37-0	128921	46	60	2	73	40	14	0	37	5375
18.	38	000123-11-5	121855	44	55	2	56	37	14	0	35	5287
19.	*38	000499-75-2	123690	39	57	2	59	37	14	11	36	5966
20.	*37	000095-16-9	121694	33	43	2	51	43	13	2	35	5872

Peak 112



Scan 751 (17.385 min): A0981.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	54	57.90	162	71.95	59	93.15	447
44.00	83	59.00	271	77.05	331	94.95	691
44.90	432	60.00	42	79.05	343	96.05	523
46.95	70	62.00	229	80.20	106	96.95	1925
49.95	246	63.00	113	81.05	380	97.95	213
50.95	338	65.00	217	82.00	217	104.95	84
51.95	146	67.00	370	83.00	598	107.00	290
53.05	371	68.00	163	83.95	101	107.90	106
55.05	419	69.00	634	86.00	89	109.00	325
56.05	140	69.95	283	91.00	285	110.00	191
56.90	112	70.80	147	92.15	109	111.00	117

Scan 751 (17.385 min): A0981.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
119.00	82	143.00	180				
120.95	165	143.95	134				
123.05	85						
124.05	223						
124.95	1187						
132.90	39						
135.00	566						
136.00	165						
137.00	593						
141.00	1217						
142.00	2643						

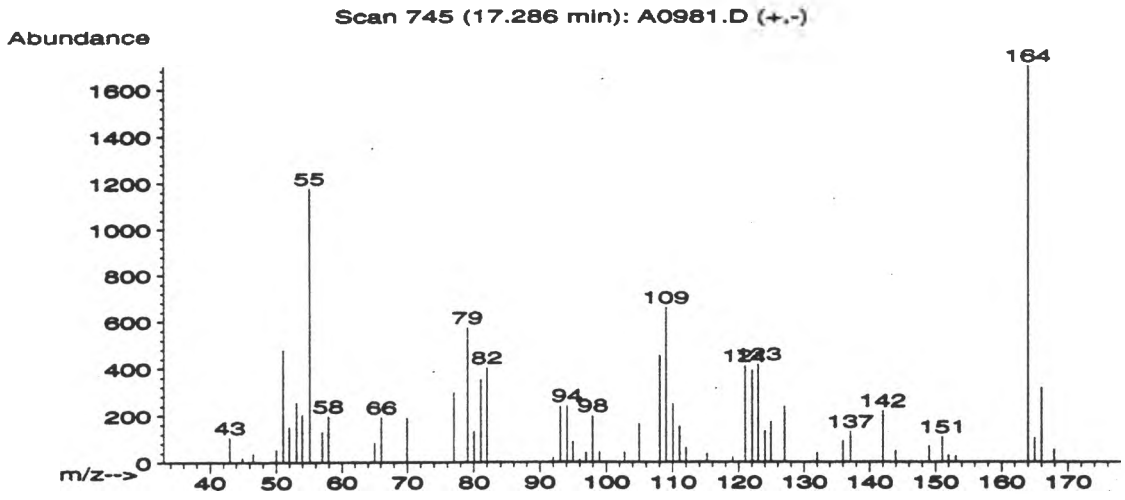
Scan 751 (17.385 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3-METHYL-2-THIOPHENECARBOXYLIC ACID	142	C6H6O2S	53
2.	2-Thiophenecarboxylic acid, 5-methyl-	142	C6H6O2S	49
3.	4-AMINO-1-METHYL-5-NITROPYRAZOLE	142	C4H6N4O2	35
4.	2-Methylthiophen-3-carboxylic acid	142	C6H6O2S	32
5.	4(1H)-Pyrimidinone, 2-(methylthio)-	142	C5H6N2OS	30
6.	2,2,4-Trimethyl-3-pentenioc acid	142	C8H14O2	30
7.	Propanedioic acid, 3-thienyl-	186	C7H6O4S	27
8.	2(1H)-Pyrimidinethione, 4,5-diamino-	142	C4H6N4S	27
9.	Cyclohexane, isocyanato-	125	C7H11NO	14
10.	4-AMINO-1-METHYL-3-NITROPYRAZOLE	142	C4H6N4O2	12
11.	1-2-D3-ETHYL-2-PYRIDTHIONE	139	C7H6D3NS	10
12.	2(1H)-Pyrimidinone, 3,4-dihydro-1-methyl	142	C5H6N2OS	10
13.	1-Azabicyclo[2.2.2]octan-3-one	125	C7H11NO	10
14.	5-AMINO-2-CHLORO-4-PICOLINE	142	C6H7ClN2	10
15.	2-PYRONE-4-D	96	C5H3DO2	10
16.	4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-	142	C6H6O4	9
17.	4H-Pyran-4-one, 5-hydroxy-2-(hydroxymeth	142	C6H6O4	9
18.	2(1H)-Pyrimidinethione, 4,6-diamino-	142	C4H6N4S	9
19.	6-Methyl-4-thiouracil	142	C5H6N2OS	9
20.	2,4-Hexadienedioic acid, (Z,Z)-	142	C6H6O4	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	000000-00-0	9792	76	35	1	81	38	28	30	59	9237
2.	*49	001918-79-2	122588	55	54	1	69	37	23	0	49	9442
3.	*35	089607-16-9	9764	36	78	3	83	53	11	0	39	8064
4.	*32	001918-78-1	9794	30	28	1	90	46	9	5	34	8789
5.	*30	005751-20-2	9783	51	38	0	82	60	9	0	46	7164
6.	*30	004177-03-1	9957	36	45	0	71	58	9	2	43	6605
7.	27	021080-92-2	28131	44	62	1	70	57	8	16	38	7587
8.	*27	014623-58-6	9768	40	54	0	79	59	8	17	40	7122
9.	*14	003173-53-3	120457	45	41	1	72	66	2	16	38	5549
10.	*12	039205-76-0	9765	36	68	2	99	65	2	2	37	7247
11.	*10	053966-48-6	8900	40	75	1	68	70	1	0	33	7316
12.	*10	035455-86-8	9781	36	46	0	93	69	1	0	35	6888
13.	*10	003731-38-2	120459	47	57	1	50	66	1	0	35	5929
14.	*10	000000-00-0	9823	41	56	2	87	70	1	6	35	6766
15.	*10	020357-67-9	553	36	59	2	107	80	1	0	41	5117
16.	* 9	001073-96-7	9814	28	73	3	97	71	1	0	33	6865
17.	* 9	000501-30-4	122592	33	67	1	76	72	1	0	35	6972
18.	* 9	001004-39-3	9769	35	56	2	91	72	1	0	35	6826
19.	* 9	000000-00-0	9782	28	45	0	78	73	1	0	33	6780
20.	9	001119-72-8	9803	55	39	1	70	76	1	0	36	5605

Peak 113



Scan 745 (17.286 min): A0981.D

Modified:added subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	106	65.05	82	95.00	87	112.00	62
44.90	19	66.10	191	95.95	11	115.15	37
46.55	37	69.95	188	96.95	42	119.05	21
50.00	53	77.00	295	97.95	197	121.00	407
51.05	477	79.05	571	98.95	42	122.05	390
51.95	150	80.05	133	102.80	42	123.00	415
53.05	254	81.05	351	105.00	165	124.00	134
53.95	202	82.00	400	108.05	452	124.95	171
55.05	1176	92.00	20	109.00	658	127.00	237
56.95	130	93.05	236	110.05	248	132.00	39
57.90	196	94.10	239	111.00	152	136.00	90

Scan 745 (17.286 min): A0981.D

Modified:added subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.10	130						
142.00	217						
143.95	49						
149.05	69						
151.05	107						
152.00	29						
153.10	25						
164.00	1699						
165.00	102						
166.00	315						
167.90	55						

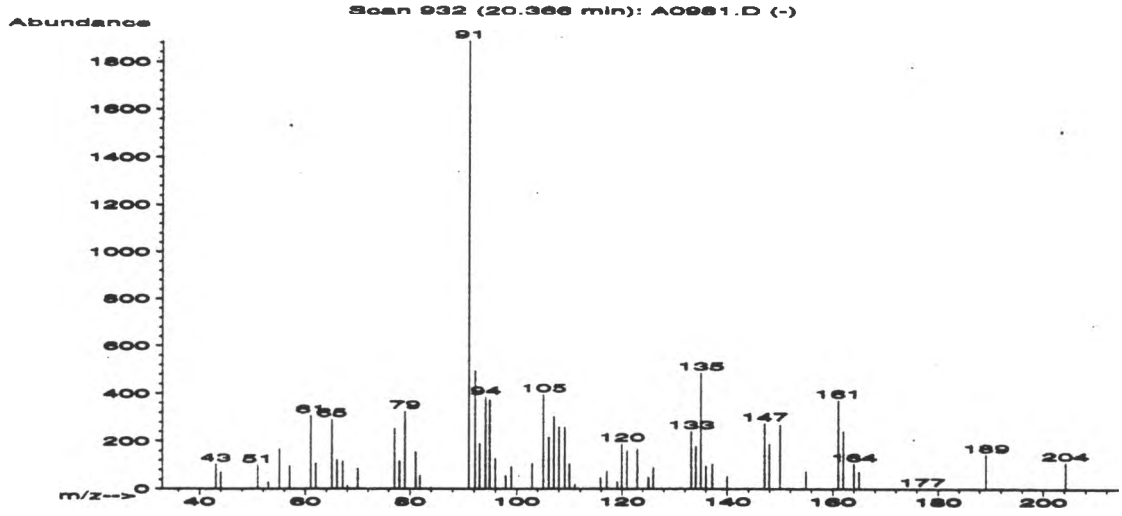
Scan 745 (17.286 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	7-Benzofuranol, 2,3-dihydro-2,2-dimethyl	164	C10H12O2	25
2.	2-Benzothiazolamine, N-methyl-	164	C8H8N2S	23
3.	2(3H)-Benzothiazolimine, 3-methyl-	164	C8H8N2S	17
4.	2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-te	164	C10H12O2	17
5.	3-Methyl-2-(trans-1-pentenyl)-2-cyclopen	164	C11H16O	12
6.	Methanimidamide, N'-(4-hydroxyphenyl)-N,	164	C9H12N2O	12
7.	7-Benzofuranol, 2,3-dihydro-2,2-dimethyl	221	C12H15NO3	12
8.	3-Pyridinecarbonitrile, 1,2-dihydro-4-me	164	C8H8N2O2	12
9.	3-Pyridinecarbonitrile, 1,2-dihydro-4-me	164	C8H8N2O2	12
10.	2(1H)-Naphthalenone, octahydro-1-methyl-	166	C11H18O	10
11.	Phenol, 2-methoxy-4-(1-propenyl)-	164	C10H12O2	10
12.	4-Penten-2-ynylamine, N,N,4-trimethyl-	123	C8H13N	10
13.	2,4(1H,3H)-Pteridinedione	164	C6H4N4O2	10
14.	Cyclopropanecarboxylic acid, 2,2-dimethy	331	C19H25NO4	9
15.	2(1H)-Naphthalenone, octahydro-8a-methyl	166	C11H18O	7
16.	2(1H)-Naphthalenone, octahydro-4a-methyl	166	C11H18O	7
17.	2(1H)-Naphthalenone, octahydro-4a-methyl	166	C11H18O	7
18.	2(1H)-Pyridinone, hydrazone, dihydrochlo	181	C5H9Cl2N3	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*25	001563-38-8	18472	40	83	2	86	52	7	0	33	8776
2.	*23	016954-69-1	18313	29	88	1	98	47	6	0	29	9104
3.	*17	014779-16-9	125264	31	68	2	99	55	3	0	29	8889
4.	*17	000527-17-3	18449	28	87	2	99	52	3	0	27	8776
5.	*12	087506-04-5	18568	30	59	2	75	64	2	1	30	7965
6.	*12	002350-51-8	18371	30	81	2	82	56	2	0	27	8557
7.	12	001563-66-2	129765	46	106	1	52	65	2	0	37	8689
8.	*12	000524-40-3	125262	34	74	2	98	65	2	0	35	8348
9.	*12	000524-40-3	18296	34	70	2	98	65	2	0	35	8348
10.	*10	021102-88-5	19646	35	73	1	41	76	1	0	39	4193
11.	*10	000097-54-1	125324	28	82	2	99	65	1	0	26	8348
12.	*10	019837-34-4	4590	40	49	0	25	80	1	0	39	3145
13.	*10	000487-21-8	125239	31	75	3	97	63	1	0	27	8448
14.	9	007696-12-0	83209	50	95	0	51	71	1	0	35	8571
15.	* 7	002530-17-8	19652	29	92	1	63	80	1	0	23	4341
16.	7	000938-07-8	125595	34	77	2	47	73	1	0	21	4105
17.	7	000938-06-7	125593	37	90	2	58	71	1	0	20	4163
18.	7	062437-99-4	25929	33	87	1	32	80	1	0	21	3504

Peak 114



Scan 932 (20.366 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	102	68.00	12	94.15	383	110.00	104
44.00	71	69.95	85	94.95	372	111.00	18
50.95	98	77.05	254	95.95	127	115.90	48
52.95	29	78.00	116	97.95	56	117.10	75
55.05	168	79.05	324	98.95	93	119.05	30
57.00	94	81.05	155	102.95	105	119.95	188
61.00	306	81.95	56	105.05	394	121.00	159
62.00	107	83.95	6	106.05	216	122.95	167
65.00	291	91.00	1885	107.00	305	125.05	48
66.00	120	92.15	494	108.00	259	125.95	87
67.10	115	93.05	190	109.10	259	133.15	241

Scan 932 (20.366 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.05	179	164.00	105				
135.00	486	165.00	72				
136.00	94	177.00	2				
137.15	102	189.15	145				
140.00	53	204.20	112				
147.05	275						
147.95	188						
150.00	268						
154.95	74						
161.00	372						
162.00	242						

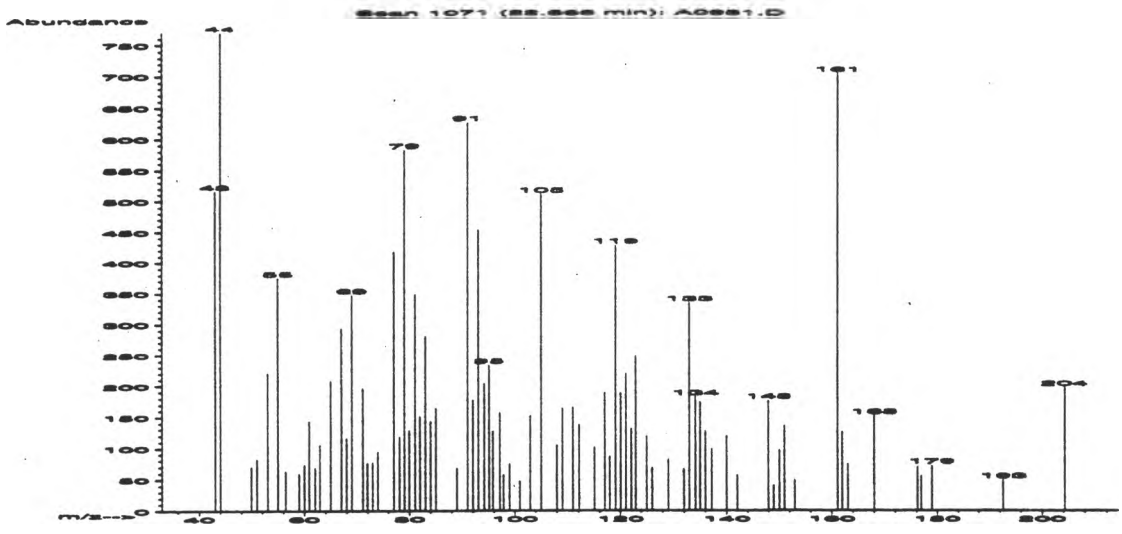
Scan 932 (20.366 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Junipene	204	C15H24	42
2.	trans-Caryophyllene	204	C15H24	27
3.	ISOCARYOPHYLLEN	204	C15H24	22
4.	2-METHYL-5,7-DIMETHYLENE-1,8-NONADIENE	162	C12H18	16
5.	(+)-Aromadendrene	204	C15H24	12
6.	Dispiro[2.1.2.4]undecane, 8-methylene-	162	C12H18	10
7.	1-(1'-Methoxycyclopropyl)-6,6-dimethyl-2	222	C14H22O2	10
8.	Z-Citral	152	C10H16O	10
9.	cis-anti-cis-Tricyclo[7.3.0.0(2,6)]-7-do	162	C12H18	10
10.	ISOCARYOPHYLLEN	204	C15H24	10
11.	Propanedinitrile, (1,2-dimethylpropylide	134	C8H10N2	10
12.	trans-Caryophyllene	204	C15H24	10
13.	Bicyclo[2.2.1]heptan-2-one, 4,7,7-trimet	167	C10H17NO	10
14.	Benzene, (1-ethyl-1-methylpropyl)-	162	C12H18	9
15.	Benzenemethanamine, N-ethyl-	135	C9H13N	9
16.	9-Octadecenoic acid, (2-phenyl-1,3-dioxo	444	C28H44O4	9
17.	2-Butanol, 4-(benzyloxy)-	180	C11H16O2	9
18.	1,2-Benzenedicarboxylic acid, bis(phenyl	346	C22H18O4	9
19.	CIS,CIS,TRANS-3,3,6,6,9,9-HEXAMETHYL-TET	204	C15H24	9
20.	4,7-Methano-1H-indene, octahydro-2-(1-me	176	C13H20	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*42	000475-20-7	128709	65	60	1	37	56	17	0	64	7574
2.	*27	000087-44-5	128693	49	88	2	51	60	8	0	39	9009
3.	*22	000118-65-0	36695	48	83	2	36	63	5	0	39	7536
4.	16	000000-00-0	17823	48	71	2	71	60	3	0	31	7066
5.	*12	000489-39-4	128755	43	81	1	37	65	2	0	35	7517
6.	10	051567-08-9	17903	34	71	1	85	70	1	8	30	5831
7.	10	091531-52-1	44861	42	72	1	19	61	1	0	29	6917
8.	10	000106-26-3	123957	43	67	2	106	66	1	0	37	6080
9.	*10	070702-18-0	17914	40	55	0	13	78	1	0	39	5912
10.	*10	000118-65-0	128696	36	65	1	19	68	1	1	30	7651
11.	*10	013017-52-2	7333	33	58	0	24	78	1	0	41	5024
12.	*10	000087-44-5	36693	41	64	0	12	80	1	5	40	7155
13.	10	004514-87-8	125663	45	68	0	26	73	1	0	39	5126
14.	* 9	001985-97-3	17837	33	58	2	128	80	1	0	35	4928
15.	* 9	014321-27-8	121746	42	71	3	92	73	1	0	35	5879
16.	9	056599-46-3	104043	46	116	1	99	76	1	0	35	6676
17.	9	004799-69-3	25611	42	64	2	99	73	1	2	31	5968
18.	9	000523-31-9	134854	46	89	3	120	80	1	0	37	5075
19.	9	000000-00-0	36802	39	73	0	34	78	1	0	33	4946
20.	9	074793-54-7	126508	44	66	1	30	80	1	0	31	6360

Peak 115



Scan 1071 (22.666 min): A0981.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	516	62.90	105	79.05	581	94.15	203
44.00	770	65.00	208	79.95	128	95.05	233
49.95	70	67.00	293	81.05	348	95.80	127
50.95	82	68.00	116	82.00	151	97.05	157
53.05	221	69.00	347	83.00	280	97.80	57
54.95	375	71.05	196	84.00	143	98.95	75
56.45	64	71.95	76	85.00	164	100.95	47
59.00	59	72.95	77	89.00	68	102.95	152
60.00	74	73.95	94	91.00	625	105.05	509
60.90	143	77.05	417	92.00	177	108.00	105
62.00	69	78.05	118	93.00	452	109.00	164

Scan 1071 (22.666 min): A0981.D

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.00	166	126.05	69	148.95	41	192.65	49
112.15	138	129.05	82	150.05	97	204.20	197
115.00	101	132.00	67	150.95	136		
117.00	189	133.00	334	152.95	49		
118.00	87	134.15	182	161.15	704		
119.05	427	135.00	174	162.00	126		
120.05	188	136.00	127	163.00	75		
121.05	220	137.15	99	168.00	152		
122.05	132	140.00	120	176.20	70		
122.95	248	142.00	57	176.95	55		
125.05	120	147.95	176	178.95	72		

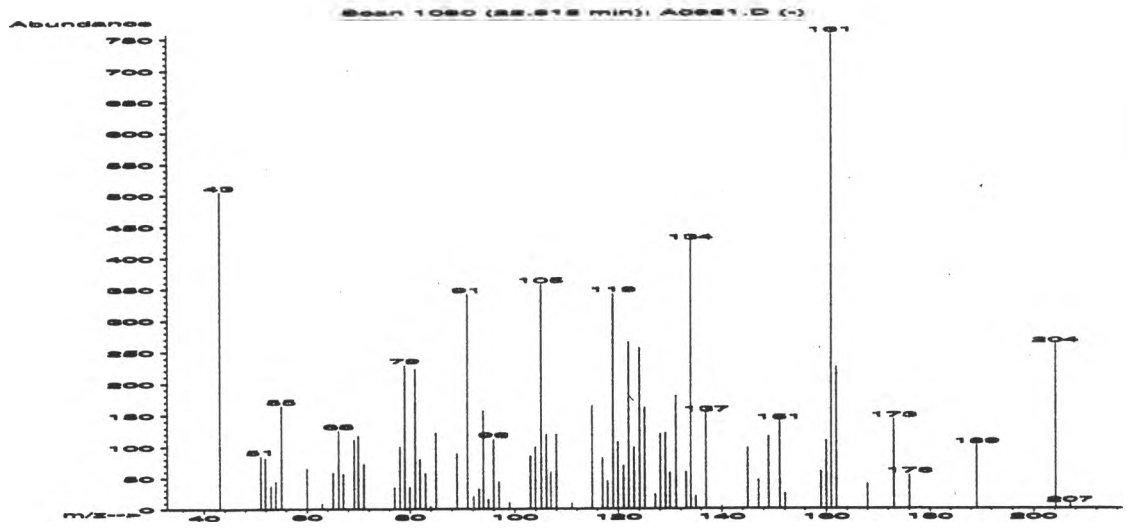
Scan 1071 (22.666 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	(+)-Aromadendrene	204	C15H24	78
2.	Junipene	204	C15H24	46
3.	.gamma.-Cadinene	204	C15H24	38
4.	(E)-Farnesene	204	C15H24	35
5.	4-Allyl-2,6-dimethylaniline	161	C11H15N	35
6.	CIS-CARYOPHYLLENE	204	C15H24	22
7.	CIS-CARYOPHYLLENE	204	C15H24	22
8.	trans-Farnesol	222	C15H26O	18
9.	s-Triazolo[1,5-a]pyridine, 2,5,7-trimeth	161	C9H11N3	14
10.	Benzene, 1-(1-ethylpropyl)-2-propyl-	190	C14H22	14
11.	Isothiazole, 4-phenyl-	161	C9H7NS	14
12.	ISOCARYOPHYLLEN	204	C15H24	14
13.	trans-Caryophyllene	204	C15H24	14
14.	Cyclopropa[d]naphthalen-2(4aH)-one, 1,1a	204	C14H20O	11
15.	exo-4-Methylbicyclo[3.2.1]octan-3-ene	122	C9H14	11
16.	3-(2-Thienyl)pyridine	161	C9H7NS	11
17.	1,3,5,8-UNDECATETRAENE	148	C11H16	10
18.	(-)-CARYOPHYLLENE OXIDE	220	C15H24O	10
19.	3-Undecen-5-yne, (E)-	150	C11H18	10
20.	trans-Caryophyllene	204	C15H24	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	000489-39-4	128755	93	69	1	63	40	46	34	83	8139
2.	*46	000475-20-7	128709	63	88	3	152	52	20	0	64	6772
3.	38	039029-41-9	128720	60	84	0	82	46	14	0	39	7210
4.	*35	000106-28-5	36637	70	70	1	150	66	11	0	76	7284
5.	*35	004494-83-1	17325	33	37	0	69	53	11	0	41	5336
6.	22	013877-93-5	36692	43	106	0	43	64	5	16	41	7202
7.	*22	013877-93-5	128685	52	99	0	43	61	5	8	41	7258
8.	18	000106-28-5	129870	78	70	1	141	66	3	0	43	7284
9.	*14	004931-30-0	17229	51	65	0	85	69	2	1	40	6207
10.	14	054789-15-0	30208	45	67	0	74	67	2	2	41	5989
11.	*14	000936-46-9	17216	37	58	0	91	69	2	0	41	5418
12.	14	000118-65-0	36695	45	109	0	59	69	2	0	39	7390
13.	*14	000087-44-5	128692	52	100	0	44	66	2	10	41	6967
14.	*11	004677-90-1	36609	50	107	3	121	76	2	0	46	6003
15.	*11	078965-86-3	4484	49	49	0	75	76	2	19	44	4241
16.	*11	069277-26-5	17219	44	56	0	91	73	2	0	44	5294
17.	*10	050277-31-1	12173	33	77	0	56	75	1	0	41	4743
18.	10	001139-30-6	129752	45	43	0	58	80	1	2	41	4241
19.	*10	074744-29-9	12909	33	78	0	75	80	1	0	41	4241
20.	*10	000087-44-5	128691	52	98	0	43	71	1	8	41	5539

Peak 116



Scan 1080 (22.815 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	505	69.10	112	85.00	122	103.95	100
51.00	85	69.95	117	89.00	89	105.05	356
51.95	82	71.00	72	91.00	340	106.05	119
53.00	37	77.05	34	92.10	20	106.95	59
53.95	44	78.05	100	93.15	32	108.00	119
55.05	164	79.05	228	94.00	157	111.00	10
60.00	65	79.95	35	95.00	16	115.00	164
62.95	9	81.05	222	95.95	112	116.95	82
65.05	58	81.95	80	97.00	44	118.00	45
66.15	125	83.00	57	99.05	11	119.05	341
67.10	56	83.95	4	103.05	85	119.95	107

Scan 1080 (22.815 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
121.05	69	134.00	425	161.00	757		
122.05	264	135.00	20	162.00	225		
123.05	99	137.00	152	168.00	39		
124.05	255	140.00	4	173.05	142		
125.05	161	144.95	98	176.05	54		
127.05	23	147.00	47	189.15	101		
128.05	120	148.95	116	204.20	260		
129.05	121	151.05	139	207.00	7		
129.95	58	152.05	24				
131.05	180	159.00	60				
133.05	60	160.00	109				

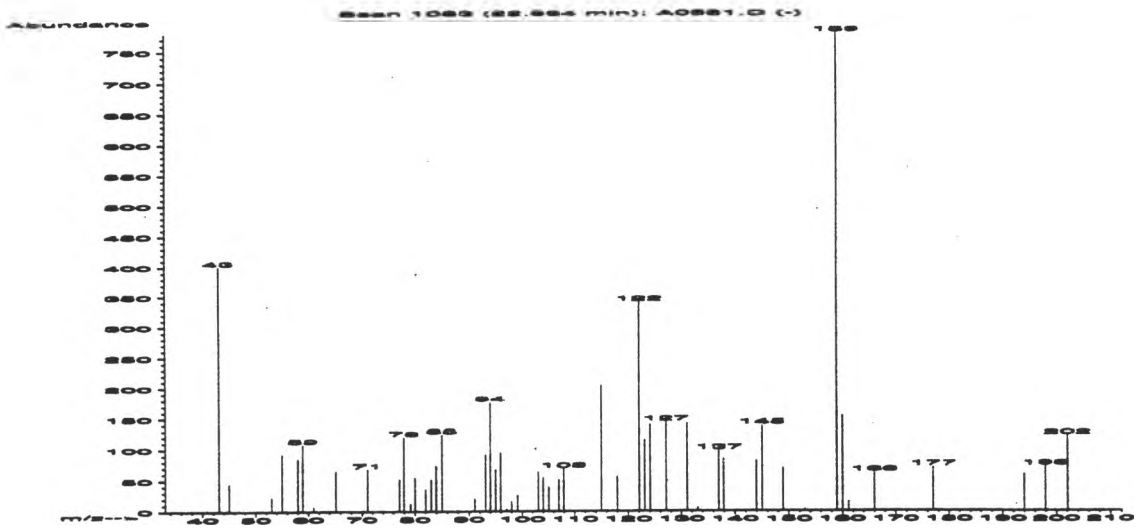
Scan 1080 (22.815 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	.delta.-Cadinene	204	C15H24	64
2.	.delta.-Cadinene	204	C15H24	60
3.	CADINENE	204	C15H24	50
4.	.delta.-Cadinene	204	C15H24	49
5.	.alpha.-Cubebene	204	C15H24	45
6.	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro	204	C15H24	38
7.	6,10,11,11-TETRAMETHYL-TRICYCLO[6.3.0.1(	204	C15H24	38
8.	Naphthalene, 1,2,3,4,4a,5,6,8a-octahydro	204	C15H24	38
9.	(E)-5-Acetyl-2,2-dimethyl-1-(3'-methyl-1	204	C14H20O	35
10.	Thiazole, 5-phenyl-	161	C9H7NS	27
11.	3a(1H)-Azulenol, 2,3,4,5,8,8a-hexahydro-	222	C15H26O	27
12.	Isothiazole, 4-phenyl-	161	C9H7NS	27
13.	Cyclohexanone, 6-furfurylidene-2,2-dimet	204	C13H16O2	25
14.	Pyrido[2,3-d]pyrimidine, 4-methoxy-	161	C8H7N3O	22
15.	1-Penten-3-one, 1-(4-methoxyphenyl)-4-me	204	C13H16O2	22
16.	(+)-Aromadendrene	204	C15H24	18
17.	(+-)-3-Isopropyl-6-methyltricyclo[4.4.0.	204	C14H20O	16
18.	EPI-BICYCLOSESQUIPHELLANDRENE	204	C15H24	15
19.	Isothiazole, 3-phenyl-	161	C9H7NS	14
20.	.alpha.-Ylangene	204	C15H24	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*64	000483-76-1	128725	69	58	2	99	35	37	0	76	9061
2.	*60	000483-76-1	128723	82	48	3	99	36	35	46	72	8976
3.	*50	000523-47-7	36723	60	75	2	94	33	25	7	40	8675
4.	*49	000483-76-1	36725	52	98	2	82	36	23	0	46	8965
5.	*45	017699-14-8	128769	65	55	1	87	48	19	29	51	7710
6.	*38	030021-74-0	36741	52	82	3	81	55	14	0	46	8410
7.	*38	000000-00-0	36805	59	87	3	85	48	14	0	41	8221
8.	*38	030021-74-0	128739	43	100	3	99	46	14	0	39	8433
9.	*35	077822-54-9	36588	37	88	2	99	53	11	0	39	8182
10.	*27	001826-13-7	17214	35	59	2	89	56	8	0	39	8069
11.	27	000465-28-1	44999	44	88	0	84	56	8	19	41	8152
12.	*27	000936-46-9	17216	52	49	1	91	56	8	7	40	7837
13.	*25	017429-54-8	36497	60	93	3	72	63	7	0	46	7486
14.	*22	028732-78-7	17153	36	72	2	74	64	5	0	39	7353
15.	*22	000103-13-9	36482	33	73	1	85	62	5	0	39	7532
16.	*18	000489-39-4	128754	52	114	3	53	70	3	0	46	8091
17.	*16	029642-55-5	36616	38	86	2	99	60	3	16	37	7659
18.	*15	000000-00-0	36657	59	60	3	189	73	2	0	51	7860
19.	*14	010514-34-8	17215	34	70	2	99	67	2	0	39	7316
20.	*12	014912-44-8	128767	49	68	1	59	63	2	12	37	7817

Peak 117



Scan 1083 (22.864 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	400	79.15	12	97.00	3	123.05	115
44.95	44	80.00	54	98.00	15	124.05	140
53.00	22	82.00	35	99.05	25	127.05	143
55.05	92	83.00	51	103.05	63	131.05	142
58.00	84	83.95	73	103.95	54	133.05	5
58.90	107	85.00	124	105.05	39	137.00	97
60.95	7	91.10	20	106.95	51	137.90	84
65.05	64	93.05	91	107.90	68	143.95	81
71.00	67	94.00	176	115.00	204	145.05	138
77.05	51	94.95	67	118.00	56	148.95	69
77.95	119	95.95	95	122.05	340	153.00	2

Scan 1083 (22.864 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
159.00	779						
160.00	154						
161.15	15						
166.00	61						
177.05	70						
193.95	59						
197.95	71						
202.05	121						

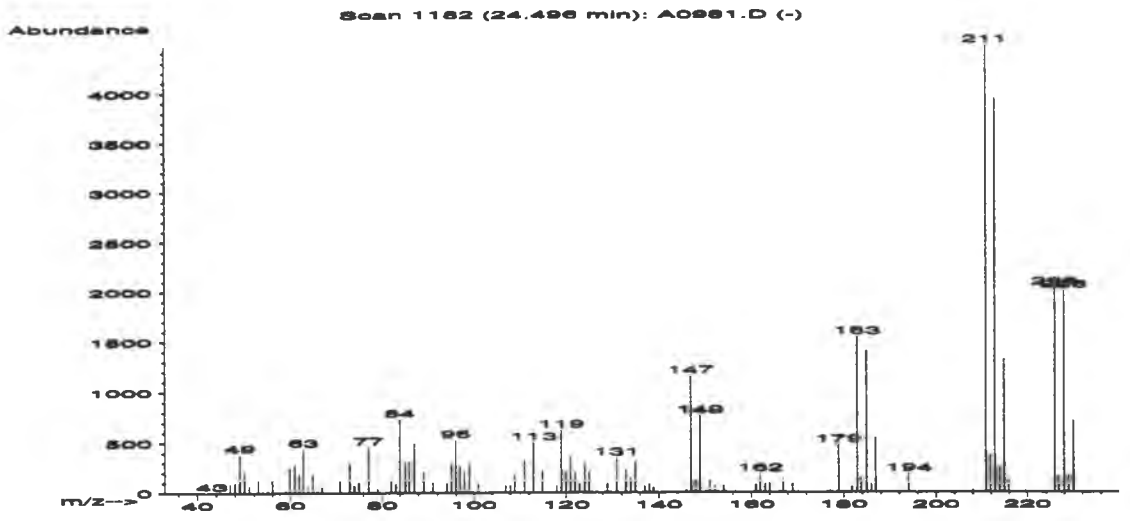
Scan 1083 (22.864 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Naphthalene, 1,2,3,4-tetrahydro-1,6-dime	202	C15H22	37
2.	2-Pyrimidinamine, 4-chloro-6-methoxy-	159	C5H6ClN3O	35
3.	1,8-Naphthyridin-2-amine, 5-methyl-	159	C9H9N3	35
4.	1,1,3,3-TETRAMETHYLINDANE	174	C13H18	32
5.	3-BENZYL-1,2,4-TRIAZOLE	159	C9H9N3	27
6.	3-BENZYL-1,2,4-TRIAZOLE	159	C9H9N3	27
7.	Oxazole, 4-methyl-5-phenyl-	159	C10H9NO	27
8.	2(1H)-Naphthalenone, octahydro-3-methyl-	166	C11H18O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*37	000483-77-2	35797	30	74	0	99	43	13	2	35	8851
2.	*35	005734-64-5	16365	33	92	1	99	53	11	0	39	8865
3.	*35	001568-92-9	16437	35	67	0	86	53	11	0	41	8699
4.	32	004834-33-7	23250	38	69	2	99	48	9	0	33	8718
5.	*27	021117-34-0	124789	35	69	1	73	60	8	0	41	8663
6.	*27	021117-34-0	16442	35	70	1	75	59	8	0	39	8740
7.	*27	001008-29-3	16496	36	69	2	79	58	8	0	39	8691
8.	7	055332-01-9	125592	39	54	1	39	74	1	0	20	4020

Peak 118



Scan 1182 (24.496 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	6	61.00	280	77.05	455	95.05	289
46.95	91	62.00	189	79.00	41	95.95	521
47.95	98	62.90	439	82.00	144	96.95	264
48.95	386	63.95	50	83.00	89	97.95	211
49.95	209	65.00	184	83.90	730	98.95	289
51.00	70	66.00	41	85.00	296	100.95	90
52.95	146	67.00	56	85.90	317	103.95	45
54.95	14	70.95	128	87.00	493	106.00	16
56.05	152	72.95	293	89.00	203	106.95	74
59.00	18	73.95	73	91.00	102	108.00	75
59.90	251	74.95	105	94.00	99	108.95	178

Scan 1182 (24.496 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
111.00	322	128.95	92	148.95	761	177.05	9
113.00	501	130.95	350	149.95	4	178.95	470
114.90	215	132.95	225	151.00	119	181.75	54
118.00	69	134.00	148	152.05	60	182.90	1538
119.00	623	135.00	309	153.95	71	183.75	142
119.95	206	137.00	62	160.95	76	184.90	1400
120.95	355	138.00	89	161.90	186	185.90	84
121.95	201	138.90	52	163.00	86	186.90	543
122.95	83	145.95	37	163.95	91	194.05	184
124.05	286	146.95	1152	166.90	132	208.00	23
125.05	203	147.95	127	168.95	84	210.90	4469

Scan 1182 (24.496 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
211.90	367						
212.90	3929						
213.90	249						
214.90	1318						
215.90	122						
225.95	2032						
226.80	161						
227.95	2002						
228.95	172						
229.95	713						

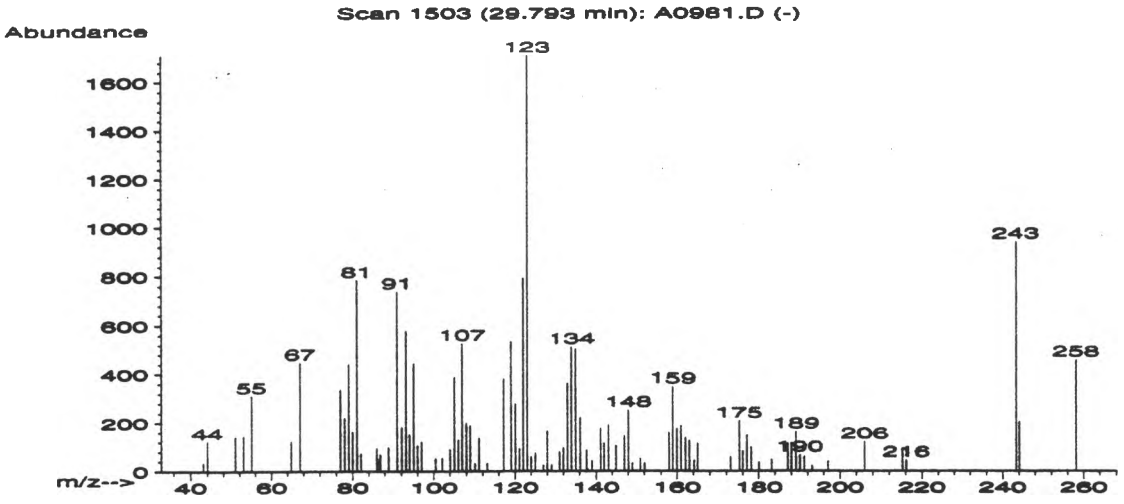
Scan 1182 (24.496 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3,4,5-Trichloroguaiacol	226	C7H5Cl3O2	97
2.	2,4-Dichloro-1-methoxy-naphthalene	226	C11H8Cl2O	46
3.	3,5,6-TRICHLORO-N-METHYL-2-PYRIDONE	211	C6H4Cl3NO	38
4.	[1,1'-Biphenyl]-2-ol, 3-(1,1-dimethyleth	226	C16H18O	16
5.	Acridine, 9-chloro-	213	C13H8ClN	14
6.	1,2,4-Thiadiazol-3-amine, 5-(2-chlorophe	211	C8H6ClN3S	14
7.	Thiazolo[5,4-d]pyrimidine, 7-(ethylthio)	211	C8H9N3S2	14
8.	Benzenamine, 2-chloro-N,N-diethyl-4-nitr	228	C10H13ClN2O2	12
9.	9H-Purine, 6-chloro-9-(trimethylsilyl)-	226	C8H11ClN4Si	9
10.	Carbamic acid, methylphenyl-, 2-chloroet	213	C10H12ClNO2	8
11.	THIAZOLO[4,5-d]PYRIMIDIN-7(6H)-ONE	213	C7H7N3OS2	8
12.	Phenol, 2-(2-benzoxazolyl)-	211	C13H9NO2	8
13.	2-METHYLTHIO-4-OXO-6-(2-THIENYL)-3,4,5,6	226	C9H10N2OS2	7
14.	Phenol, 4,4'-(1-methylethylidene)bis-	228	C15H16O2	7
15.	Benzothiazole, 2-phenyl-	211	C13H9NS	7
16.	1-Dodecanamine, N-methyl-N-nitroso-	228	C13H28N2O	7

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*97	057057-83-7	46362	89	29	0	84	0	78	0	95	9424
2.	*46	000000-00-0	46462	57	79	1	56	41	20	0	47	9423
3.	*38	000000-00-0	39760	48	66	1	75	38	14	0	37	8918
4.	*16	002416-98-0	46944	30	89	3	87	58	3	3	30	7140
5.	*14	001207-69-8	40803	35	99	3	87	70	2	0	39	5759
6.	*14	042053-84-9	39775	35	111	1	74	67	2	0	39	7773
7.	*14	055030-64-3	39781	33	120	2	70	68	2	0	39	7046
8.	12	000086-49-7	47430	33	126	2	87	60	2	0	22	6369
9.	* 9	032865-86-4	46386	36	84	2	36	76	1	0	35	8097
10.	* 8	055030-68-7	40723	30	120	3	70	70	1	0	29	5777
11.	* 8	000000-00-0	40681	32	105	2	69	68	1	0	23	5933
12.	* 8	000835-64-3	39910	30	82	3	81	69	1	0	27	6655
13.	* 7	000000-00-0	46402	32	93	2	45	73	1	0	27	6748
14.	7	000080-05-7	47751	38	78	1	74	73	1	0	28	5961
15.	* 7	000883-93-2	39919	31	82	3	96	74	1	0	29	6518
16.	7	055090-44-3	47638	34	103	3	85	76	1	0	20	6252

Peak 119



Scan 1503 (29.793 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	32	80.00	162	95.05	444	110.10	31
44.00	122	81.05	782	96.05	105	111.15	137
50.95	142	82.00	73	97.05	122	113.10	33
53.00	144	86.00	95	100.45	53	117.15	381
54.00	3	86.50	48	102.05	54	119.00	534
55.05	311	86.90	68	104.05	90	120.05	278
65.00	122	88.90	98	105.05	385	121.05	93
67.10	448	91.00	736	106.05	129	122.05	793
77.00	336	92.10	180	107.00	527	123.05	1711
78.05	220	93.15	577	108.00	198	124.05	59
79.05	440	94.05	151	109.00	188	125.05	75

Scan 1503 (29.793 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
127.05	25	139.00	43	159.00	349	178.20	98
128.00	167	141.15	176	160.00	175	180.05	36
129.05	26	142.00	115	161.00	186	183.15	47
131.00	79	143.15	190	162.10	138	187.15	115
132.00	96	145.00	104	163.00	126	188.00	116
133.00	363	147.00	144	164.15	44	189.15	163
134.00	513	148.05	252	165.05	114	190.10	67
135.00	504	149.05	33	173.00	59	191.10	60
136.10	220	151.00	53	175.20	208	193.05	20
137.65	85	152.05	32	176.05	83	197.05	40
138.00	6	158.00	159	177.05	148	206.05	122

Scan 1503 (29.793 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
208.90	2						
215.15	87						
216.15	46						
243.25	939						
244.05	202						
258.15	459						

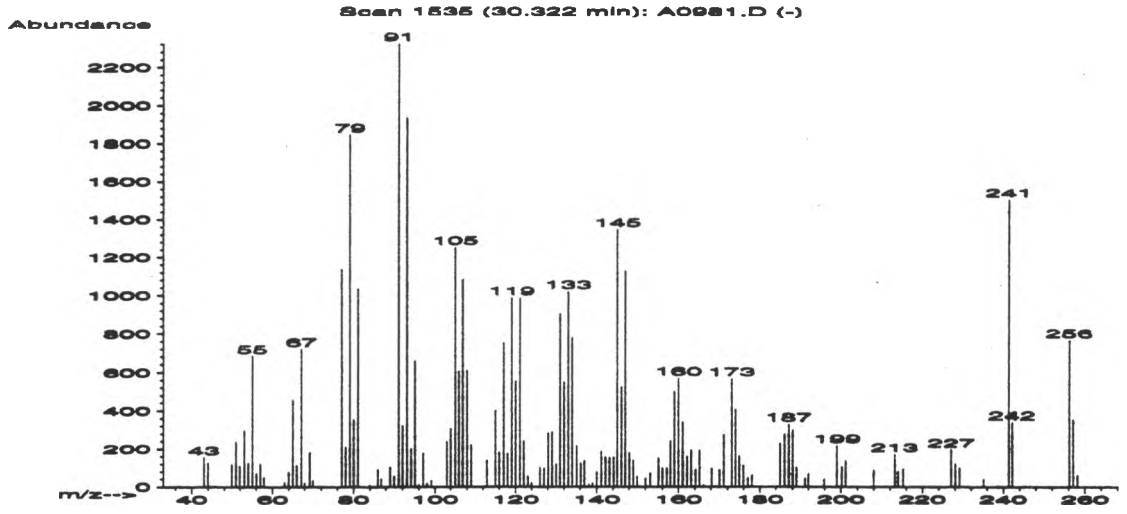
Scan 1503 (29.793 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-METHYLSULFONYL-P-METHOXYACETANILIDE	243	C10H13NO4S	32
2.	Phenol, 3-amino-2-methyl-	123	C7H9NO	27
3.	Phenol, 4-amino-3-methyl-	123	C7H9NO	27
4.	exo-8-Bromo-2-oxatricyclo[3.3.0.0(4,6)]o	202	C7H7BrO2	25
5.	Pyrethrin I	328	C21H28O3	10
6.	PHOTONEROL A	154	C10H18O	10
7.	1,4-Hexadiene, 2,3,4,5-tetramethyl-	138	C10H18	10
8.	trans-DL-Chrysanthemumic acid	168	C10H16O2	10
9.	Ethyl chrysanthemumate	196	C12H20O2	10
10.	Cyclopropanecarboxylic acid, 2,2-dimethy	342	C21H26O4	10
11.	Cyclopropanecarboxylic acid, 2,2-dimethy	302	C19H26O3	10
12.	Allethrine	302	C19H26O3	10
13.	TRANS-10-METHYLDECALONE-1	166	C11H18O	9
14.	5-ISOPROPENYL-3,3,4,5-TETRAMETHYL-1,2-OX	202	C10H18O2S	9
15.	3a,6-Epoxy-3aH-isoindole, 1,2,3,6,7,7a-h	243	C15H17NO2	9
16.	METHYL ESTER OF O-PHENOXY CARBANILIC ACI	243	C14H13NO3	9
17.	cis-Chrysanthemic acid	168	C10H16O2	9
18.	3a,6-Epoxy-3aH-isoindole, 1,2,3,6,7,7a-h	243	C15H17NO2	9
19.	2,5-Heptadien-4-one, 2,6-dimethyl-	138	C9H14O	9
20.	Bicyclo[2.2.2]octane, 1-iodo-4-methyl-	250	C9H15I	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	32	064856-19-5	53601	44	112	3	92	48	9	0	31	8556
2.	*27	053222-92-7	4586	35	60	2	83	58	8	0	39	7856
3.	*27	002835-99-6	120311	44	62	2	74	58	8	0	39	7809
4.	25	000000-00-0	35242	69	69	1	86	51	7	0	37	8130
5.	10	000121-21-1	82395	39	101	1	70	68	1	5	33	7295
6.	10	060619-35-4	14638	45	46	2	93	71	1	17	38	7206
7.	10	051504-54-2	8754	47	57	2	99	70	1	2	37	7264
8.	10	000705-16-8	20340	46	53	1	88	70	1	1	35	7324
9.	10	000097-41-6	32943	53	68	2	95	70	1	0	36	7261
10.	10	055622-64-5	86118	42	103	2	99	68	1	10	31	6972
11.	10	028434-00-6	74631	54	88	3	97	70	1	10	37	7236
12.	10	000584-79-2	74615	46	104	3	99	68	1	0	35	7407
13.	9	000000-00-0	19656	43	60	2	72	71	1	10	37	7194
14.	9	000000-00-0	35387	41	72	2	70	72	1	4	31	7138
15.	* 9	017960-79-1	53720	40	83	2	48	77	1	4	37	4669
16.	* 9	000000-00-0	53696	39	102	2	38	79	1	0	35	4442
17.	9	015259-78-6	20339	45	66	2	76	71	1	0	37	7210
18.	* 9	071840-23-8	53721	40	80	1	44	79	1	8	37	4428
19.	* 9	000504-20-1	8597	33	65	1	77	71	1	0	35	7184
20.	9	055044-63-8	56144	53	77	3	99	72	1	18	37	7138

Peak 120



Scan 1535 (30.322 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	155	63.00	21	80.00	356	95.05	658
44.00	128	64.00	78	81.05	1033	96.05	11
49.95	118	65.05	456	84.00	7	97.05	177
50.95	239	66.00	113	86.00	92	98.00	18
51.95	110	67.15	721	86.90	42	99.05	32
53.00	297	68.00	19	89.00	106	103.00	239
54.00	125	69.15	181	90.00	56	103.95	307
55.05	684	69.95	34	91.05	2322	105.05	1249
56.05	71	77.05	1136	92.05	324	106.05	605
57.00	122	78.05	211	93.10	1928	107.00	1081
57.90	49	79.05	1846	94.10	201	108.00	610

Scan 1535 (30.322 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
109.05	221	124.05	21	136.10	127	147.05	1125
113.00	140	126.05	102	137.00	138	148.05	180
115.00	400	127.05	97	138.15	13	149.05	140
116.00	182	128.10	284	139.00	19	150.00	53
117.05	751	129.05	287	140.00	78	152.00	44
118.00	175	130.05	121	141.15	187	153.05	70
119.05	985	131.05	902	142.15	157	155.05	151
119.95	553	132.00	548	143.10	153	156.05	100
121.05	984	133.00	1017	144.20	155	157.15	99
122.05	242	134.00	779	145.05	1343	158.00	242
123.05	56	135.10	216	146.05	524	159.00	500

Scan 1535 (30.322 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
160.00	570	173.05	568	191.15	43	228.05	122
161.05	342	174.05	406	192.00	69	229.20	100
162.10	161	175.00	162	195.80	38	235.15	39
163.15	193	175.95	113	199.05	218	241.25	1504
164.15	91	177.05	45	200.20	106	242.15	341
165.15	193	178.05	61	201.20	136	256.15	768
166.15	8	185.00	230	208.00	90	257.15	355
168.15	98	186.15	277	213.15	173	258.15	61
169.05	3	187.15	330	214.00	81		
170.05	90	188.15	298	215.15	94		
171.05	276	189.10	102	227.05	197		

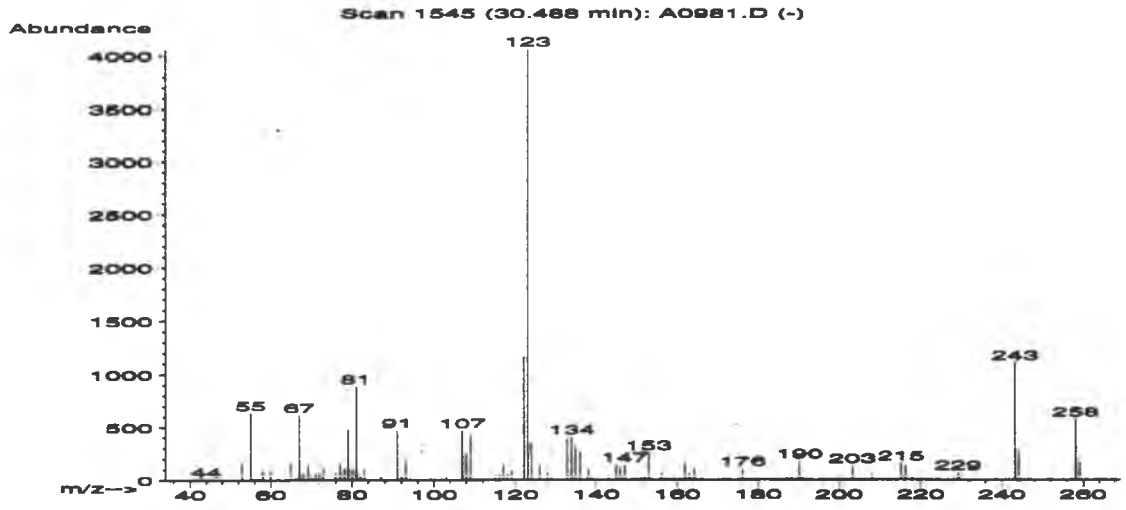
Scan 1535 (30.322 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclohexane, 1,5-diethenyl-3-methyl-2-me	162	C12H18	53
2.	Mixture of trans,trans-1,3-Dimethylenecy	188	C14H20	41
3.	Cholic acid	408	C24H40O5	38
4.	trans-Caryophyllene	204	C15H24	38
5.	1,7-OCTADIENE, 2,7-DIMETHYL-3,6-DIMETHYL	162	C12H18	35
6.	CIS/TRANS-7-BICYCLO[4.1.0]HEPT-7-YLIDENE	188	C14H20	35
7.	1,5-Hexadiene, 2,5-dimethyl-3-methylene-	122	C9H14	25
8.	CYCLOPENTAN-3'-SPIROTRICYCLO[3.1.0.0(2,4	188	C14H20	25
9.	3-Methylene-1,6-hexadiene	108	C8H12	22
10.	2-CARENE, 4-.ALPHA.-ISOPROPENYL-, (+)-	176	C13H20	22
11.	Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyd	150	C10H14O	15
12.	2-PHENYL-1-BROMOETHANE-2,2-D2	184	C8H7D2Br	15
13.	Carbonic dihydrazide, 2,2'-diphenyl-	242	C13H14N4O	15
14.	3-Tetradecen-5-yne, (Z)-	192	C14H24	15
15.	3-Tetradecen-5-yne, (E)-	192	C14H24	15
16.	1H-Pyrrole, 3-ethyl-5-[(4-ethyl-3,5-dime	256	C17H24N2	11
17.	CYCLOPENTANE, 1-METHYLEN-2-VINYL-	108	C8H12	11
18.	Camphene	136	C10H16	10
19.	.alpha.-Sinensal	218	C15H22O	10
20.	Bicyclo[3.1.1]hept-2-ene-2-carboxaldehyd	150	C10H14O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	074742-35-1	17868	79	53	1	60	39	28	38	58	7708
2.	*41	066405-18-3	29413	58	28	0	92	52	16	0	56	7758
3.	38	000081-25-4	136142	81	88	3	90	50	14	23	40	7296
4.	38	000087-44-5	128695	62	80	3	117	50	14	0	39	7622
5.	*35	000000-00-0	17825	64	51	0	68	54	11	8	43	7036
6.	*35	000000-00-0	29441	70	73	1	70	69	11	0	76	6666
7.	*25	059131-13-4	4462	71	36	1	79	65	7	6	47	6697
8.	*25	078578-93-5	29438	63	80	1	77	63	7	0	50	6406
9.	22	016626-48-5	1950	44	56	0	63	64	5	6	41	6446
10.	22	000000-00-0	24060	53	58	0	54	63	5	7	40	6636
11.	*15	000564-94-3	12850	58	56	1	54	73	2	0	56	5116
12.	*15	015785-29-2	27235	60	50	0	79	72	2	0	56	5614
13.	*15	000140-22-7	53260	68	63	0	56	80	2	15	58	5169
14.	*15	074663-68-6	31087	62	65	1	56	76	2	0	56	6629
15.	*15	074744-44-8	31088	62	66	0	54	76	2	0	56	6643
16.	*11	002407-83-2	59075	48	100	1	64	80	2	0	44	4090
17.	*11	006196-78-7	118756	57	51	0	66	72	2	7	46	6593
18.	*10	000079-92-5	122049	35	77	1	81	73	1	20	40	6473
19.	10	017909-77-2	129600	44	85	0	58	71	1	10	41	7162
20.	10	023727-16-4	12849	73	46	1	58	71	1	0	41	5817

Peak 121



Scan 1545 (30.488 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	6	70.05	37	83.00	91	114.95	44
52.95	169	71.05	54	87.00	33	116.00	50
55.05	631	71.95	58	91.00	465	117.00	146
56.00	15	72.95	120	92.10	48	118.00	54
58.00	87	75.95	62	93.00	176	119.05	90
59.90	82	77.05	150	97.05	2	122.05	1162
65.00	169	78.05	109	99.05	11	123.05	4053
66.10	20	79.05	475	103.05	51	124.00	350
67.00	611	80.05	99	107.00	461	126.05	140
68.00	56	81.05	880	108.00	243	128.05	63
69.15	138	82.00	39	109.00	416	129.00	32

Scan 1545 (30.488 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
133.00	387	151.05	18	187.10	21	217.90	35
134.05	401	152.05	33	188.15	41	229.20	65
135.00	320	152.95	252	190.15	174	243.25	1103
136.15	265	156.05	71	191.00	22	244.20	271
138.15	101	159.10	15	198.00	7	258.15	567
139.05	24	162.00	159	201.05	10	259.15	159
143.10	41	163.10	51	203.20	129		
145.05	133	164.20	108	205.20	10		
145.95	120	166.00	12	208.00	51		
147.05	141	176.20	101	215.15	151		
150.05	24	179.05	2	216.25	133		

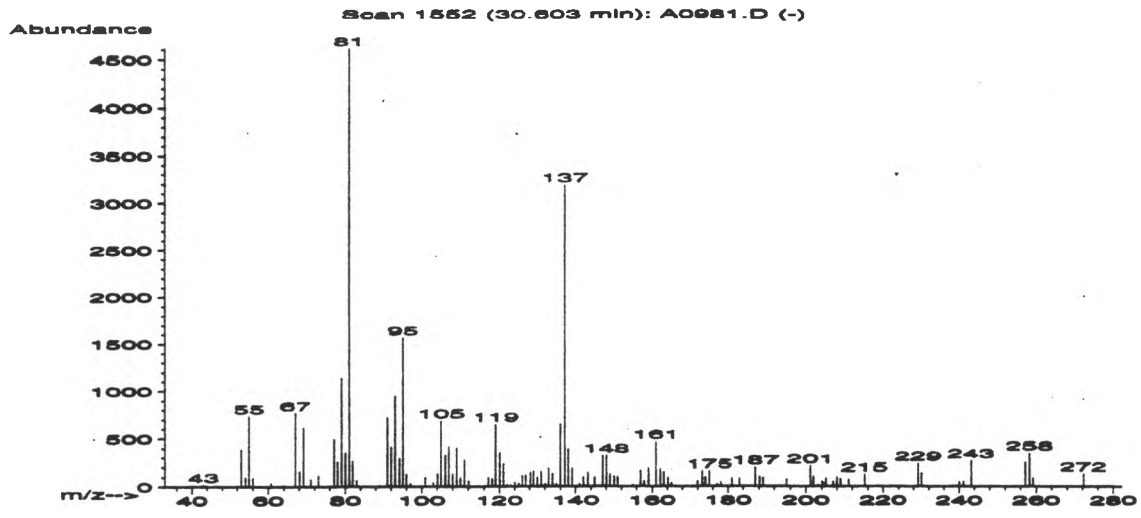
Scan 1545 (30.488 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Jasmolin I	330	C21H30O3	40
2.	D1-2-4-HYDROXY-3-METHYL-2-CYCLOPENTEN-1-	302	C19H26O3	37
3.	Allethrine	302	C19H26O3	37
4.	Cinerin I	316	C20H28O3	37
5.	Phenol, 3-amino-2-methyl-	123	C7H9NO	37
6.	3-Furancarboxamide, 2,5-dimethyl-N-pheny	215	C13H13NO2	35
7.	4,4'-ISOPROPYLIDENE DICYCLOHEXANOL	240	C15H28O2	28
8.	Pyrethrin I	328	C21H28O3	25
9.	1,2,3,3,4-PENTAMETHYL-CYCLOPENTENE	138	C10H18	25
10.	(3E)-4-(1,2-Epoxy-2,6,6-trimethylcyclohe	252	C15H24O3	25
11.	2-Pyrimidinamine, N,N-dimethyl-	123	C6H9N3	25
12.	Phenol, 4-amino-2-methyl-	123	C7H9NO	25
13.	Benzenamine, 3-methoxy-	123	C7H9NO	25
14.	4-Pyridinecarboxylic acid	123	C6H5NO2	25
15.	(+)-(4aR,6R,8aR)-6-Isopropenyl-4,8a-dime	218	C15H22O	23
16.	3-Heptyne, 5,5-diethyl-	152	C11H20	23
17.	Benzenemethanol, .alpha.-(aminomethyl)-4	153	C8H11NO2	23
18.	Furan, 2-(1,1-dimethylethyl)-4-methyl-	138	C9H14O	17
19.	Pyridine, 3-ethyl-, 1-oxide	123	C7H9NO	17
20.	Ethyl chrysanthemumate	196	C12H20O2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	40	004466-14-2	134458	53	83	3	73	33	16	2	30	9436
2.	37	000137-98-4	74622	53	81	2	69	44	13	11	31	8837
3.	37	000584-79-2	133547	58	76	2	66	44	13	8	35	8838
4.	37	025402-06-6	134031	47	102	3	82	44	13	0	37	9270
5.	*37	053222-92-7	4586	34	60	1	71	44	13	0	35	9352
6.	*35	028562-70-1	129404	39	51	2	92	55	11	18	40	9063
7.	28	000000-00-0	52670	39	64	1	90	38	8	0	28	9436
8.	25	000121-21-1	82395	39	109	3	78	44	7	0	24	9141
9.	25	000000-00-0	8771	41	43	1	70	54	7	6	31	9091
10.	25	084114-01-2	57347	36	25	1	78	44	7	0	22	9142
11.	*25	005621-02-3	4537	29	88	3	99	41	7	0	29	9405
12.	*25	002835-96-3	4588	28	73	1	85	43	7	0	27	9410
13.	*25	000536-90-3	4583	28	41	1	90	55	7	6	35	9052
14.	*25	000055-22-1	4520	30	71	0	85	54	7	0	33	9058
15.	23	086917-82-0	129614	41	63	2	83	50	6	0	29	9094
16.	23	061228-06-6	13862	34	68	2	77	50	6	0	25	9296
17.	*23	004502-14-1	14024	30	85	1	118	50	6	0	29	9087
18.	17	006141-68-0	8606	39	42	2	82	55	3	0	22	9037
19.	*17	014906-62-8	120307	28	90	2	95	55	3	0	29	8947
20.	10	000097-41-6	32943	43	74	1	50	69	1	0	35	9170

Peak 122



Scan 1552 (30.603 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	22	73.05	114	93.00	949	108.00	133
53.00	390	77.05	493	94.10	294	109.00	403
54.05	95	78.05	260	95.05	1566	110.00	90
55.00	736	79.05	1144	95.95	130	111.00	273
56.05	92	80.05	355	97.05	31	112.05	59
60.75	34	81.05	4609	100.95	97	117.10	91
63.95	9	82.00	264	102.95	40	118.10	82
67.00	771	83.00	63	104.05	132	119.00	651
68.10	160	88.95	15	105.00	689	120.05	353
69.05	618	91.00	723	106.05	326	121.05	238
71.05	79	92.05	415	107.00	414	122.00	20

Scan 1552 (30.603 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
123.05	12	134.00	139	147.05	321	163.10	150
124.05	48	135.00	27	148.05	324	164.15	88
125.05	34	136.05	655	149.00	128	165.10	36
126.05	114	137.15	3178	150.05	104	171.95	59
127.00	118	138.15	391	151.05	98	173.20	160
128.15	151	139.15	191	155.05	13	174.05	96
129.05	161	141.00	26	157.00	166	175.05	160
130.05	97	142.00	95	157.90	58	177.05	25
131.05	157	143.15	148	159.10	190	178.05	45
132.05	28	144.95	97	161.00	467	181.00	85
133.00	191	146.05	4	162.15	182	183.00	82

Scan 1552 (30.603 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
187.10	200	207.00	51	258.25	351		
188.15	106	208.00	103	259.15	84		
189.10	92	208.90	78	272.20	134		
192.10	6	211.00	72				
195.05	70	215.15	127				
201.20	215	229.20	243				
202.05	101	230.20	142				
203.20	12	240.00	46				
204.20	52	241.15	52				
204.55	37	243.15	268				
205.20	85	257.15	253				

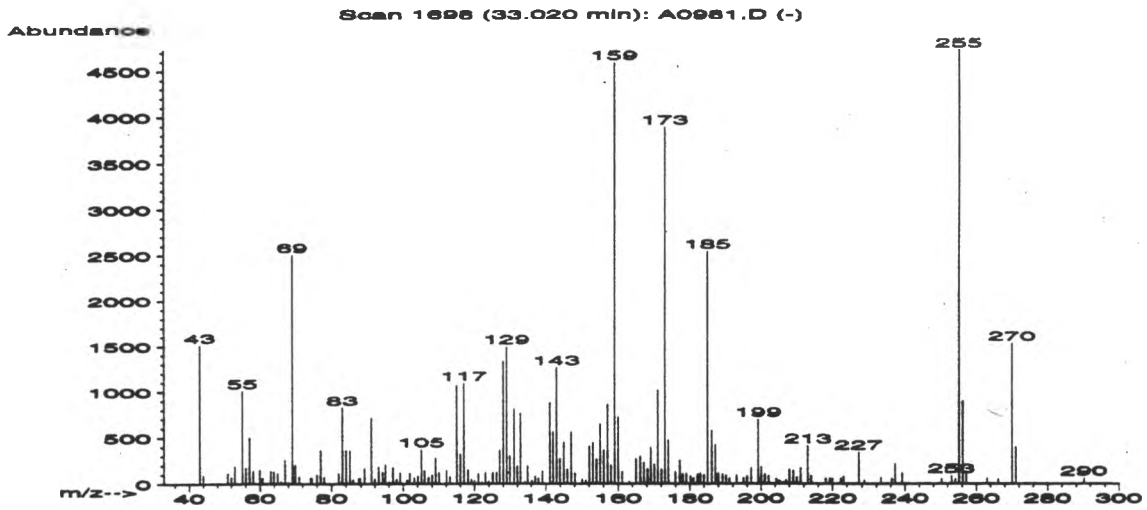
Scan 1552 (30.603 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-DEUTERIOFORMYL-2-METHOXYBENZENE	136	C8H7DO2	53
2.	NERONE	194	C13H22O	53
3.	BORNYL ESTER OF 3-ISOPROPYLIDENE-CYCLOPE	290	C19H30O2	50
4.	Phosphonous dichloride, (1,7,7-trimethyl	238	C10H17Cl2P	42
5.	PHOSPHINE, BORNYLDICHLORO-	238	C10H17Cl2P	42
6.	Cyclopentane, 1,3-dimethyl-2-(1-methylet	138	C10H18	35
7.	Cyclohexene, 3-(2-propynyl)-	120	C9H12	35
8.	CYCLOPENTANE, 1-ISOBUTYLIDEN-3-METHYL-	138	C10H18	32
9.	Bicyclo[2.1.0]pentane-5-carboxylic acid,	154	C9H14O2	25
10.	Furan, 2-pentyl-	138	C9H14O	16
11.	Bicyclo[2.2.1]heptan-2-ol, 1,3,3-trimeth	196	C12H20O2	16
12.	.beta.-Bourbonene	204	C15H24	16
13.	4,t-5-Dimethyl-c-2-(2'-methyl-1'-propeny	206	C14H22O	12
14.	1-Propanone, 2-methyl-1-(octahydro-3a-me	208	C14H24O	12
15.	1-Propanone, 2-methyl-1-(octahydro-3a-me	208	C14H24O	12
16.	Benzeneacetic acid, .alpha.-(acetyloxy)-	238	C12H14O5	10
17.	BUTANE, 1,2-DIDEUTERO-2-(P-ANISYL)-	164	C11H14D2O	10
18.	1-Buten-1-ol, 2-methyl-4-(2,6,6-trimethy	236	C15H24O2	10
19.	Benzaldehyde, 3-hydroxy-, oxime	137	C7H7NO2	10
20.	1H-Pyrrole-2-carboxylic acid, 1-ethenyl-	137	C7H7NO2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*53	013278-00-7	7798	33	34	0	56	29	28	9	38	5415
2.	53	031375-17-4	32031	55	59	0	71	28	28	19	41	9289
3.	50	000000-00-0	70699	57	97	3	79	17	25	6	37	9563
4.	42	074630-16-3	51405	45	71	2	94	27	17	0	37	9694
5.	42	000000-00-0	51406	45	71	2	94	27	17	0	37	9694
6.	*35	061142-31-2	8781	34	68	2	97	54	11	11	40	7902
7.	*35	055956-43-9	4149	50	34	1	99	54	11	10	39	7774
8.	32	000000-00-0	8779	46	61	2	88	49	9	0	35	8144
9.	25	074810-55-2	14460	43	48	2	75	54	7	0	37	7767
10.	*16	003777-69-3	122265	38	41	1	81	60	3	3	36	7671
11.	16	076109-40-5	33038	44	76	3	95	56	3	5	37	7899
12.	16	005208-59-3	128770	43	80	3	77	56	3	0	35	7537
13.	12	092356-17-7	37607	47	89	1	57	63	2	0	37	6191
14.	12	066708-25-6	128997	43	54	1	52	63	2	0	37	9464
15.	12	066708-25-6	38720	43	54	1	52	63	2	0	37	9464
16.	10	055538-79-9	51490	43	62	0	63	79	1	19	41	5265
17.	10	000000-00-0	18598	44	38	1	65	79	1	16	41	5269
18.	10	021730-91-6	50874	56	56	0	68	71	1	2	41	5846
19.	*10	022241-18-5	8270	33	52	0	52	73	1	0	41	5808
20.	*10	034600-55-0	8233	35	81	2	68	67	1	0	35	5619

Peak 82



Scan 1698 (33.020 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1509	63.00	138	76.05	99	91.00	709
44.00	91	63.90	130	77.00	363	92.00	50
50.95	113	65.00	112	78.00	73	93.10	184
51.95	70	66.00	26	82.00	114	94.15	127
53.00	190	67.05	258	83.00	824	95.05	203
55.05	1007	68.00	14	84.00	359	96.05	21
56.05	177	69.15	2501	85.10	356	97.05	174
57.00	498	70.00	204	85.95	43	98.05	46
58.00	136	71.05	78	87.50	54	99.05	121
59.90	153	74.20	64	87.75	56	101.00	38
60.75	59	74.55	61	89.00	163	101.80	118

Scan 1698 (33.020 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
103.05	65	116.00	319	127.05	362	138.00	61
104.05	80	117.00	1088	128.05	1328	139.05	138
105.05	369	118.15	150	129.05	1491	141.15	874
105.95	145	119.05	46	129.95	301	142.00	559
107.00	70	120.00	31	131.05	810	143.00	1257
108.00	95	121.05	108	132.00	195	143.95	273
109.05	277	122.05	18	133.00	766	145.05	452
110.05	124	123.05	120	134.15	20	146.05	158
112.10	143	124.05	26	135.00	199	147.05	559
113.10	79	125.05	119	136.15	33	148.05	116
115.00	1063	126.10	122	137.05	81	150.05	46

Scan 1698 (33.020 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
151.05	35	163.10	24	175.00	3	186.15	576
152.05	405	165.00	272	175.95	129	187.15	423
153.10	446	166.15	298	177.20	256	188.00	117
154.05	268	167.15	234	178.05	110	189.15	105
155.05	646	168.15	162	179.05	114	190.15	96
156.05	365	169.05	393	180.15	84	191.10	61
157.15	855	170.05	211	181.05	65	193.15	91
158.00	201	171.05	1016	182.15	106	195.05	59
159.00	4588	172.05	160	183.00	118	196.05	86
160.00	727	173.05	3882	184.00	97	197.20	173
161.10	133	174.05	477	185.00	2536	199.20	694

Scan 1698 (33.020 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

200.05	185	211.15	174	236.25	57	270.05	1527
201.05	105	213.15	409	237.15	215	271.20	396
202.20	85	214.15	87	239.15	117	290.15	61
203.20	2	218.15	60	250.30	54		
204.30	54	219.30	61	253.05	86		
205.15	31	219.95	57	254.20	49		
206.10	9	222.20	57	255.20	4729		
207.00	39	223.05	80	256.15	893		
208.00	156	227.20	341	257.15	134		
209.00	141	228.70	36	263.00	56		
210.00	69	233.25	66	266.15	48		

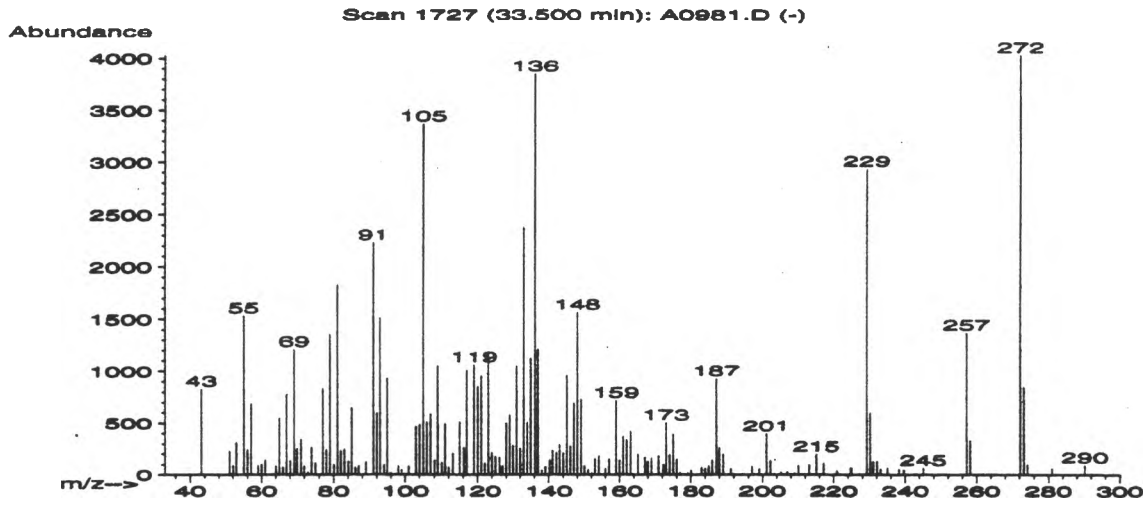
Scan 1698 (33.020 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenanthrene, 1,2,3,4,4a,9,10,10a-octahy	270	C20H30	86
2.	O-TERT-BUTYLPHENOXY)BENZOIC ACID	270	C17H18O3	74
3.	Phenanthrene, 1,2,3,4,4a,9,10,10a-octahy	270	C20H30	59
4.	Cleistantha-8,11,13-triene	270	C20H30	58
5.	Phenanthrene, 1,2,3,4,4a,9,10,10a-octahy	270	C20H30	30
6.	1-Phenanthrenecarboxaldehyde, 1,2,3,4,4a	284	C20H28O	30
7.	s-Indacene-1,7-dione, 2,3,5,6-tetrahydro	270	C18H22O2	22
8.	Naphthalene, 1,2,3,4-tetrahydro-1,5,7-tr	174	C13H18	20
9.	1-Naphthalenol, 2-nitroso-	173	C10H7NO2	14
10.	Naphthalene, 1,2,3,4-tetrahydro-2,5,8-tr	174	C13H18	14
11.	1,8-Naphthyridin-2-amine, 5,7-dimethyl-	173	C10H11N3	11
12.	2(5H)-Furanone, 5-(phenylimino)-	173	C10H7NO2	11
13.	4-piperidino-2-(2-hydroxyphenyl)pyrimidi	255	C15H17N3O	11
14.	1H-Inden-1-one, 2,3-dihydro-3,3,6-trimet	174	C12H14O	10
15.	1,3,5-Trisilacyclohexane, 1,1,3-trimethy	174	C6H18Si3	10
16.	1H-Inden-1-one, 2,3-dihydro-3,3,5,7-tetr	188	C13H16O	10
17.	2(5H)-Furanone, 5-(phenylimino)-	173	C10H7NO2	10
18.	2-Chloromethyl-5,6-dimethylbenzimidazole	194	C10H11ClN2	10
19.	4-NITRO-4'-METHOXYSTILBENE	255	C15H13NO3	10
20.	.alpha.-D-Galactopyranoside, methyl 2-(a	393	C16H35NO6Si2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	019407-28-4	132235	98	67	1	93	28	53	0	90	9642
2.	*74	069737-65-1	63630	31	12	0	98	0	44	4	37	5768
3.	*59	019407-28-4	132234	54	12	0	87	21	33	6	39	8629
4.	*58	088399-25-1	63779	59	32	0	94	33	32	0	56	9345
5.	*30	019407-28-4	63774	50	87	1	87	60	9	0	44	8397
6.	30	024035-50-5	68666	79	85	1	92	56	9	0	43	7042
7.	*22	055591-16-7	63721	63	85	2	96	64	5	18	40	5847
8.	*20	021693-55-0	23264	66	52	3	96	66	4	27	56	5718
9.	*14	000132-53-6	22603	37	84	3	61	70	2	0	39	5003
10.	14	030316-17-7	126401	58	79	2	84	70	2	0	39	5873
11.	*11	039565-07-6	22612	34	57	2	62	79	2	4	43	4507
12.	*11	019990-26-2	126255	59	63	1	82	73	2	0	46	4896
13.	*11	075634-06-9	58531	34	92	3	99	78	2	10	43	5582
14.	*10	054484-71-8	23182	36	65	1	69	76	1	20	40	5566
15.	*10	018339-88-3	22728	37	74	1	67	75	1	0	39	6360
16.	*10	054789-23-0	29366	49	60	1	61	73	1	17	39	4945
17.	*10	019990-26-2	22595	44	74	2	82	73	1	0	40	4870
18.	10	079091-12-6	31648	43	53	3	69	79	1	0	39	5327
19.	*10	000000-00-0	58519	42	26	0	75	77	1	3	38	5490
20.	10	056196-93-1	96628	74	69	1	56	75	1	1	39	5030

Peak 83



Scan 1727 (33.500 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.10	827	65.00	547	77.05	835	89.00	123
51.05	226	66.00	75	78.05	242	91.00	2226
52.05	89	67.00	773	79.05	1351	92.00	596
53.00	313	68.05	136	80.05	97	93.05	1509
55.05	1531	69.15	1208	81.05	1828	94.15	95
56.05	242	70.00	251	82.00	231	95.05	931
57.00	687	71.05	339	83.00	244	96.05	16
59.00	88	71.95	86	84.10	129	98.05	86
60.00	101	73.00	20	85.00	647	99.05	45
61.00	140	73.95	266	85.95	69	100.95	84
64.00	82	75.00	113	86.90	85	103.05	465

Scan 1727 (33.500 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
104.05	484	116.15	260	128.05	500	139.10	81
105.05	3357	117.00	1009	129.05	576	140.25	141
106.05	508	119.00	1061	130.05	286	141.05	235
107.00	585	120.05	852	131.05	1052	142.15	213
108.10	140	121.05	956	132.00	253	143.00	290
109.05	1050	122.05	112	133.00	2372	144.05	210
110.10	118	123.05	1183	134.00	505	145.05	957
111.00	489	124.05	210	135.00	1121	146.05	276
112.00	71	125.05	176	136.15	3840	147.05	692
113.15	204	126.20	166	137.00	1210	148.05	1565
115.00	512	127.05	86	138.10	42	149.05	731

Scan 1727 (33.500 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
150.05	87	163.15	414	177.05	18	191.10	58
151.05	50	165.15	196	178.05	3	197.05	80
152.15	15	167.15	171	179.10	14	199.05	56
153.05	153	168.00	128	180.10	44	201.05	397
154.20	182	168.95	157	183.00	72	202.20	137
156.00	58	170.95	180	184.00	57	205.15	20
157.05	154	172.20	97	185.00	85	207.00	25
159.00	720	173.05	505	186.00	141	209.00	13
160.00	142	174.05	191	187.15	931	210.15	90
161.00	367	175.05	391	188.00	259	213.15	94
162.00	337	176.00	147	189.10	195	215.15	198

Scan 1727 (33.500 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.

217.15	111	239.65	42
220.95	36	245.05	65
224.70	63	257.15	1371
224.95	61	258.15	332
229.20	2925	272.20	4030
230.20	599	273.20	846
231.05	125	274.20	100
232.15	130	281.05	62
233.15	54	290.25	92
235.00	63		
238.25	54		

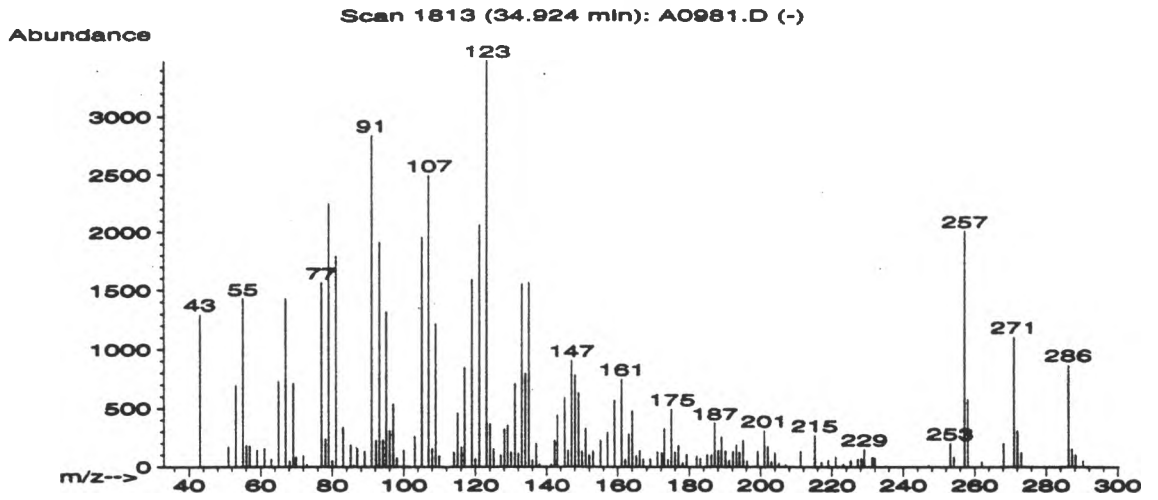
Scan 1727 (33.500 min): A0981.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	5 .ALPHA.-ANDROST-7-EN-17-ONE	272	C19H28O	49
2.	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	43
3.	Kaur-16-ene, (8.beta.,13.beta.)-	272	C20H32	43
4.	Benz[a]anthracene-5,6-diol, 5,6-dihydro-	290	C20H18O2	41
5.	Perylene, eicosahydro-	272	C20H32	30
6.	12-O-METHYLPODOCARPINAL	272	C18H24O2	27
7.	6-METHYL-4,5-DIPHENYL-4H-CYCLOPENTA[B]FU	272	C20H16O	25
8.	Estra-1,3,5(10)-triene-3,17-diol (17.bet	272	C18H24O2	22
9.	9H-Xanthen-9-one, 1,6-dihydroxy-3-methox	272	C15H12O5	18
10.	Androst-5-en-4-one	272	C19H28O	18
11.	4H-Naphtho[2,3-b]pyran-4-one, 5,6-dihydr	272	C15H12O5	14
12.	Methanone, diphenyl-, phenylhydrazone	272	C19H16N2	11
13.	ANISOLE, O-ISOPROPENYL-	148	C10H12O	11
14.	Bicyclo[2.2.1]heptane, 7-methylene-2-(1-	148	C11H16	11
15.	Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O	11
16.	1,2,3,4-Phenazinetetrol, 7,8-dimethyl-	272	C14H12N2O4	11
17.	Adamantane	136	C10H16	11
18.	3-P-TOLYLPROPANAL	148	C10H12O	11
19.	Naphthalene-d8	128	C10D8	11
20.	BUTENYL BUTENYLPHENYL ETHER	202	C14H18O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	063568-59-2	64399	49	17	0	72	36	23	0	46	5997
2.	*43	020070-61-5	64458	92	98	2	78	45	18	2	43	7979
3.	*43	020070-61-5	132290	45	148	3	120	45	18	0	40	7893
4.	*41	028622-94-8	70722	60	100	1	91	54	16	0	56	7147
5.	*30	047041-72-5	132296	69	92	2	82	62	9	0	53	7312
6.	*27	016826-83-8	64355	64	100	2	99	60	8	0	41	6901
7.	*25	086738-92-3	64430	49	98	3	79	64	7	0	46	6581
8.	*22	000050-28-2	132265	47	120	3	99	64	5	0	40	6327
9.	*18	003569-83-3	64176	48	94	1	99	67	3	0	46	6303
10.	*18	013583-72-7	64398	87	80	2	93	66	3	19	43	6034
11.	*14	003567-00-8	64178	36	98	1	99	68	2	0	41	6388
12.	*11	000574-61-8	64386	55	95	2	95	71	2	0	49	5899
13.	*11	000000-00-0	12036	49	57	0	57	78	2	0	46	3924
14.	*11	066929-97-3	12140	49	55	0	67	78	2	0	46	3920
15.	*11	000122-03-2	123389	58	59	2	66	78	2	0	46	3917
16.	*11	023774-09-6	64141	52	98	2	81	71	2	0	44	6088
17.	*11	000281-23-2	8192	49	69	0	66	78	2	0	46	5307
18.	*11	000000-00-0	12014	61	66	2	56	78	2	0	46	3927
19.	*11	000000-00-0	6077	36	50	2	95	77	2	4	43	5361
20.	*10	000000-00-0	35702	36	62	0	46	77	1	0	41	3935

Peak 86



Scan 1813 (34.924 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1296	68.15	52	85.05	187	98.05	75
50.95	169	69.15	713	86.00	14	100.00	140
53.05	699	70.00	84	86.90	155	103.05	262
55.05	1428	72.00	96	89.00	130	105.05	1950
56.05	182	72.95	23	91.00	2835	107.00	2486
57.00	177	77.05	1566	92.15	224	108.00	153
59.00	140	78.10	239	93.10	1910	109.00	1214
61.00	155	79.05	2249	94.10	228	110.00	91
63.00	68	80.05	54	95.05	1315	114.00	123
65.00	727	81.05	1791	96.05	309	115.00	460
67.00	1430	83.00	339	97.05	534	116.10	167

Scan 1813 (34.924 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
117.05	849	130.00	126	143.00	445	157.15	293
119.05	1590	131.05	709	145.05	592	159.05	568
120.05	66	132.00	115	146.05	138	161.10	748
121.05	2058	133.00	1552	147.05	906	162.10	64
123.05	3476	134.00	797	148.05	781	163.05	282
124.05	367	135.00	1569	149.05	632	164.10	479
125.05	153	136.00	60	150.00	132	165.15	95
126.05	3	137.10	201	151.05	328	166.15	140
127.05	101	138.00	27	152.05	97	167.15	67
128.05	321	141.15	22	153.10	134	169.00	71
129.00	354	142.15	225	155.20	224	171.00	128

Scan 1813 (34.924 min): A0981.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
172.20	118	186.15	104	199.20	133	218.95	59
172.95	327	187.10	376	201.05	312	221.05	87
174.05	63	188.10	140	202.05	172	223.15	26
175.05	494	189.00	255	203.05	46	225.20	56
176.00	124	190.15	134	204.05	116	227.20	66
177.00	180	191.15	56	205.10	30	228.20	72
178.05	34	192.15	130	206.05	4	229.05	151
179.15	107	193.15	188	207.00	18	231.25	81
182.00	92	194.05	126	211.15	135	232.00	76
183.10	72	195.05	228	215.15	272	235.15	4
185.00	107	196.20	52	217.15	43	247.10	18

Scan 1813 (34.924 min): A0981.D

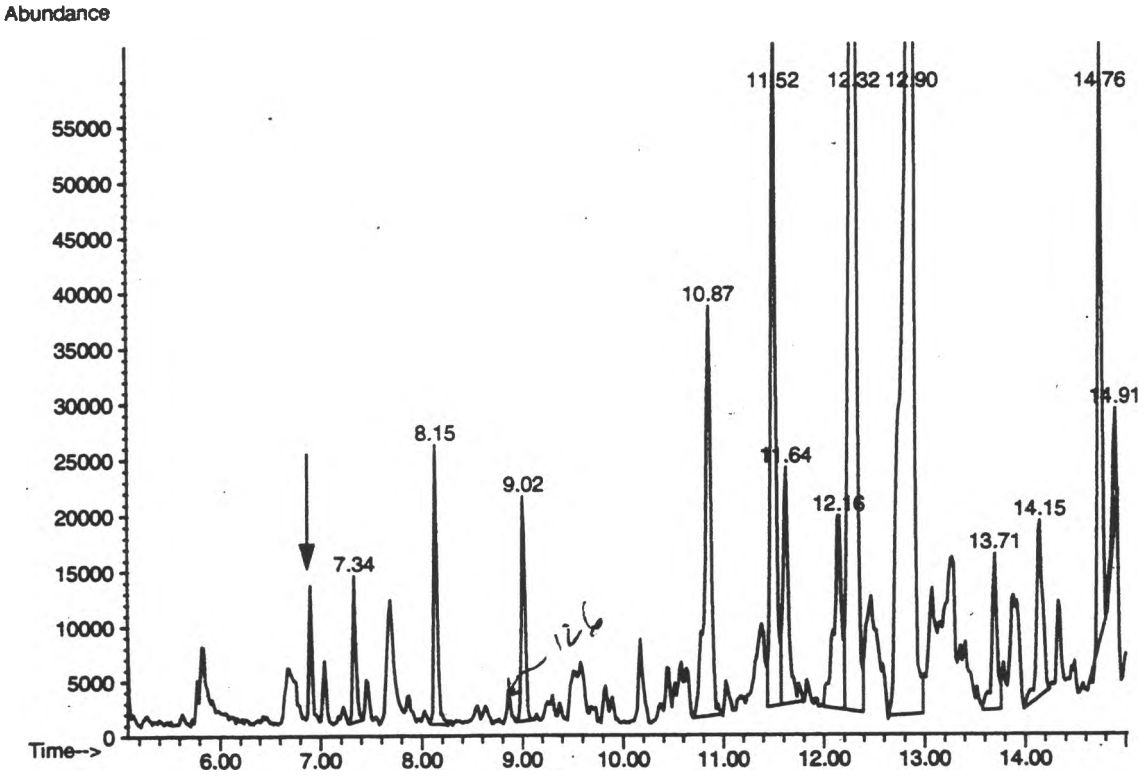
Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
253.15	202	288.15	102				

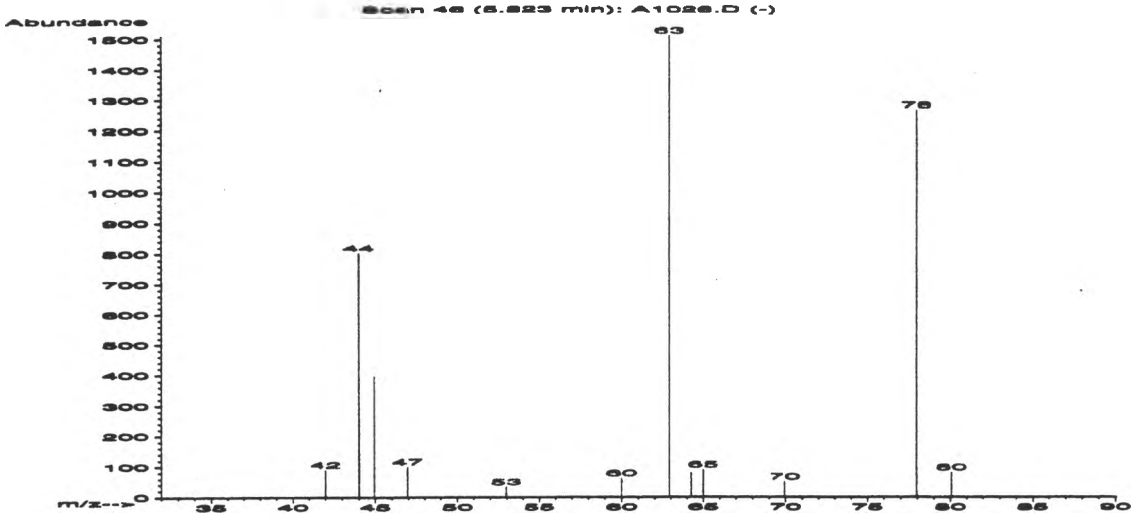
```
   254.20         87   290.25         54
   257.15       2007
   258.15        579
   262.00         44
   268.15        199
   271.05       1105
   272.05        307
   273.20        124
   286.15        871
   287.15        154
Scan 1813 (34.924 min): A0981.D


PBM Search of library D:\DATABASE\WILEY138.L

    Name                                          MolWt Formula             Qual
 1. Pimarinal                                       286 C20H30O               83
 2. (+)-VERTICILLOL                                 290 C20H34O               42
 3. Pregn-14-ene, (5.beta.)-                        286 C21H34                15
 4. Cembrene                                        272 C20H32                15
 5. VULGAROL A                                      220 C15H24O               14
 6. PIMARA-8(9),15-DIENE                            272 C20H32                14
 7. Ethaneperoxoic acid, 1-cyano-1-(4-fluoro        223 C11H10FNO3            14
 8. Trachylobane                                    272 C20H32                12
 9. Naphthalene, decahydro-1,1,4a-trimethyl-        272 C20H32                11
10. Benzenemethanol, .alpha.-(aminomethyl)-4        153 C8H11NO2              11
11. (R)-(-)-Cembrene                                272 C20H32                10
12. 4-Iodobis(bicyclo[2.2.1])hexane                 288 C12H17I               10
13. METHYL ESTER OF 4-HYDROXY-MANDELIC ACID         182 C9H10O4               10
14. (E)-3-(4-METHYL-3-CYCLOHEXENYL)BUT-2-ENY        228 C11H17Br              10
15. 1-Naphthalenepropanol, .alpha.-ethenylde        306 C20H34O2              10
16. PHOTONEROL A                                    154 C10H18O               10
17. PHOTOCITRAL A                                   152 C10H16O               10
18. TRICYCLO[3.1.0.0(2,4)]HEXANE, 3,6-DIETHY        164 C12H20                10
19. 8-ETHYLCYCLO-OCTA-2,4,6-TRIENONE                148 C10H12O               10
20. trans-Caryophyllene                             204 C15H24                10

   Prob    CAS#        Ref#    K  dK Flag   %  Con C_1 Tilt R_IV  XCORR
 1.*83 000472-39-9    69377 107  76    1  75   11  50    5   51   8590
 2.*42 070000-19-0    70756 101  59    1  41   57  17   41   80   5454
 3.*15 054411-80-2    69411  62  98    2 130   77   2    0   56   4962
 4.*15 001898-13-1   132282  72  77    2  54   76   2   28   50   4397
 5. 14 011056-03-4    44015  58  80    3 164   67   2    0   39   6266
 6.*14 018319-61-4    64465  57  82    0  42   68   2    5   38   6641
 7. 14 058422-79-0    45192  43  27    0  75   70   2    0   39   6091
 8. 12 005282-35-9    64471  45 151    2  60   62   2    0   37   8594
 9.*11 000511-02-4    64454  53 112    0  32   72   2   11   46   5320
10.*11 004502-14-1    14024  35  55    0  76   75   2    4   43   6384
11. 10 079355-93-4    64435  43 109    3  54   69   1    0   37   6288
12. 10 085407-69-8    69713  71  37    0  60   71   1   23   38   4050
13. 10 000000-00-0    26393  44  64    1  75   75   1   18   38   6284
14. 10 070240-38-9    47498  52  31    0  61   77   1   17   38   3866
15. 10 004549-12-6    75934  43 123    2  96   68   1    0   37   6502
16. 10 060619-35-4    14638  44  54    0  93   77   1    0   39   6091
17.*10 055253-27-5    13632  42  45    0  85   77   1    0   39   6091
18.*10 078578-91-3    18768  56  60    2  65   75   1   17   39   5301
19.*10 061775-57-3    12053  34  37    1  62   77   1    0   39   3884
20.*10 000087-44-5   128690  64  83    2  86   77   1    2   39   5383
```

BKME Supplimental [4]

TIC: A1026.D



Peak 123



Scan 46 (5.823 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	89	80.05	81				
44.00	801						
44.95	396						
46.95	99						
52.95	33						
60.00	62						
62.90	1511						
64.25	80						
65.00	89						
69.95	50						
77.95	1263						

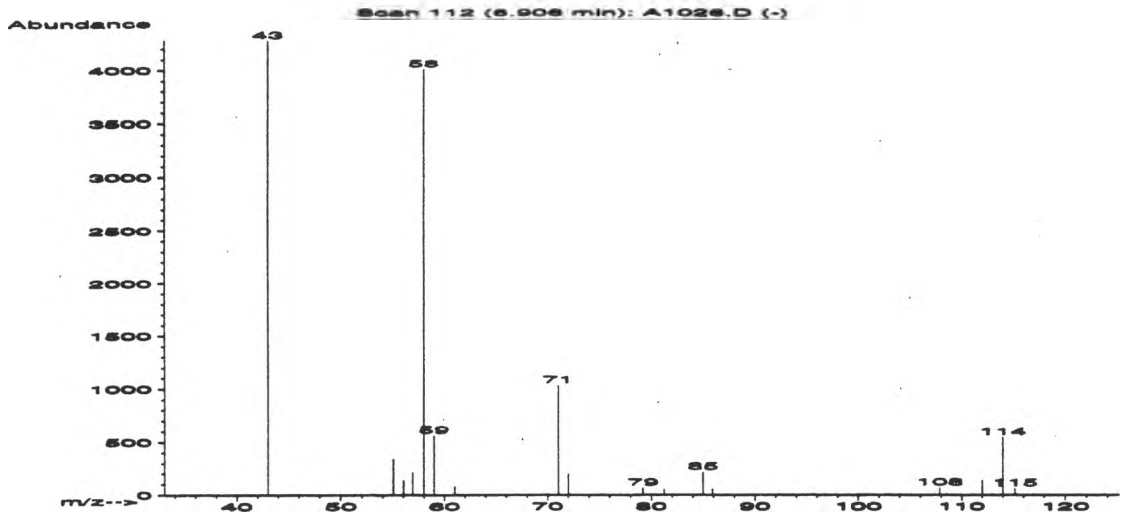
Scan 46 (5.823 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Methane, sulfinylbis-	78	C2H6OS	86
2.	Methane, sulfinylbis-	78	C2H6OS	78

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	000067-68-5	116669	34	74	0	99	8	53	4	43	9268
2.	*78	000067-68-5	116671	35	68	1	90	6	46	0	39	9320

Peak 124



Scan 112 (6.906 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4278	81.20	54				
55.05	338	85.00	215				
56.05	133	85.90	54				
56.90	215	107.90	66				
58.00	4001	112.00	136				
59.00	559	114.00	541				
61.00	80	115.15	61				
69.95	11						
71.05	1030						
72.05	197						
79.20	64						

Scan 112 (6.906 min): A1026.D

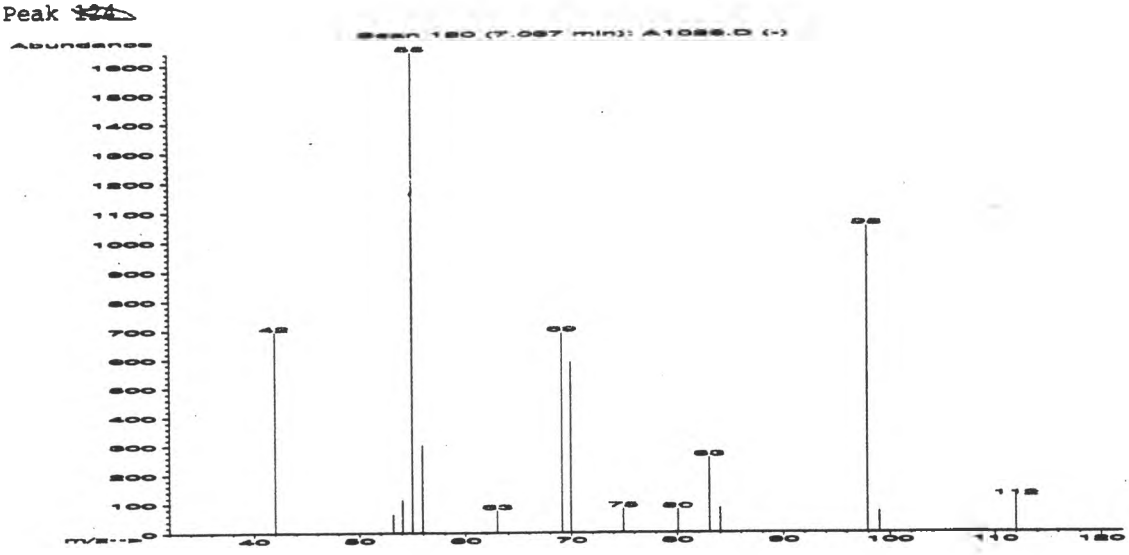
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-Heptanone	114	C7H14O	91
2.	2-Heptanone	114	C7H14O	90
3.	2-Heptanone	114	C7H14O	90
4.	2-Heptanone	114	C7H14O	83
5.	2-Heptanone	114	C7H14O	83
6.	2-Heptanone	114	C7H14O	83
7.	2-Heptanone	114	C7H14O	83
8.	2-Hexanone, 5-methyl-	114	C7H14O	72
9.	2-Heptanone	114	C7H14O	64
10.	2-Heptanone	114	C7H14O	64
11.	2-Undecanone	170	C11H22O	50
12.	Cyclohexane, 1,3-dimethoxy-, cis-	144	C8H16O2	39
13.	Undecanone	170	C11H22O	39
14.	2-Undecanone	170	C11H22O	39
15.	2-Undecanone	170	C11H22O	39
16.	2-Octanone	128	C8H16O	39
17.	2-Octanone	128	C8H16O	25
18.	3-Oxetanol, 2,2,3-trimethyl-	116	C6H12O2	17
19.	OXETANE, 2-HYDROXY-1,1,2-TRIMETHYL-	116	C6H12O2	17
20.	Butane, 2-(ethenyloxy)-2-methyl-	114	C7H14O	16

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000110-43-0	119304	63	24	0	92	4	60	10	56	9918
2.	*90	000110-43-0	119301	52	31	0	99	4	57	0	46	9883
3.	*90	000110-43-0	119305	64	23	0	82	3	57	7	47	9853
4.	*83	000110-43-0	119302	59	25	0	90	4	50	1	41	9547
5.	*83	000110-43-0	119300	55	28	0	88	4	50	3	38	9813
6.	*83	000110-43-0	3090	60	26	0	88	4	50	1	41	9665
7.	*83	000110-43-0	119299	60	25	0	87	4	50	12	41	9551
8.	*72	000110-12-3	119324	36	52	3	76	14	42	11	40	9592
9.	*64	000110-43-0	119298	47	36	1	137	17	37	0	40	9750
10.	64	000110-43-0	119303	52	34	0	71	7	37	1	36	9888
11.	50	000112-12-9	125967	33	56	2	95	17	25	2	30	9873
12.	39	030363-81-6	10743	36	69	2	71	20	15	0	22	6796
13.	39	053452-70-3	21629	34	59	1	75	19	15	0	21	9908
14.	39	000112-12-9	125963	34	59	1	75	19	15	0	21	9908
15.	39	000112-12-9	21599	33	54	1	81	19	15	0	21	9872
16.	39	000111-13-7	120849	33	57	0	86	17	15	0	25	9895
17.	25	000111-13-7	120852	33	49	1	93	42	7	0	25	9667
18.	17	025910-96-7	3477	35	55	1	83	52	3	0	25	9201
19.	17	000000-00-0	3473	35	55	1	83	52	3	0	25	9207
20.	*16	029281-39-8	3150	38	54	1	90	58	3	0	33	7411

125

Peak ~~124~~



Scan 120 (7.037 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	692	84.00	84				
53.20	62	97.95	1045				
54.05	112	99.05	72				
54.95	1642	112.00	116				
55.95	300						
63.00	74						
69.15	688						
69.95	587						
74.95	80						
80.05	77						
83.00	256						

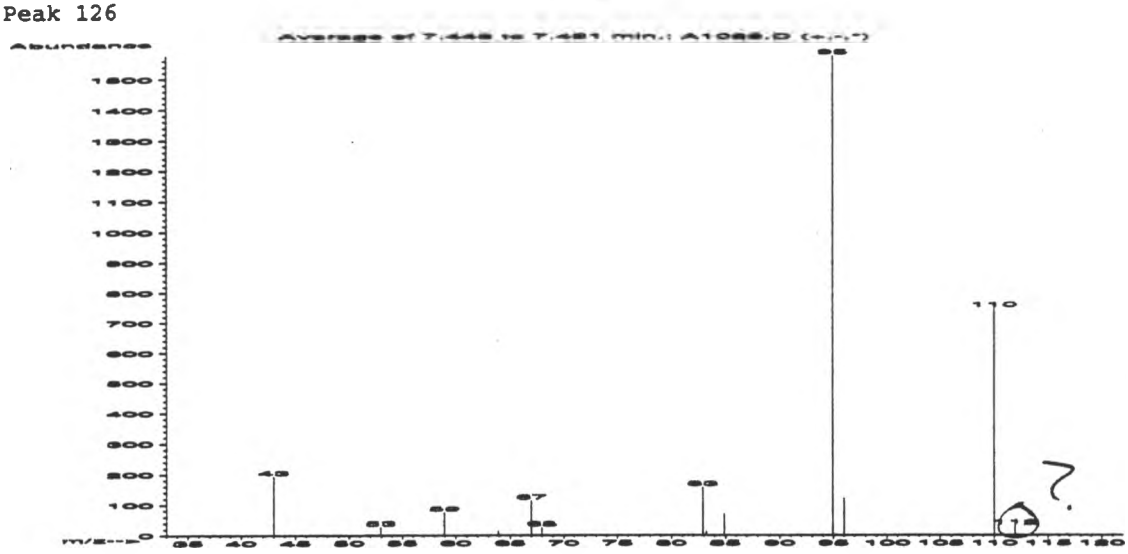
Scan 120 (7.037 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Cyclohexanone	98	C6H10O	78
2.	Cyclohexanone	98	C6H10O	78
3.	Cyclohexanone	98	C6H10O	72
4.	.GAMMA.-PICOLINE-.ALPHA.,.OMEGA.-D5	93	C6H2D5N	59
5.	Cyclohexanone	98	C6H10O	56
6.	3-Heptene	98	C7H14	50
7.	Cyclohexanone	98	C6H10O	47
8.	1,3-Cyclopentanedione	98	C5H6O2	45
9.	2(3H)-Furanone, 5-methyl-	98	C5H6O2	43
10.	Cyclohexanone	98	C6H10O	43
11.	4-PENTYNOIC ACID	98	C5H6O2	40
12.	2-Furanmethanol	98	C5H6O2	40
13.	2-Furanmethanol	98	C5H6O2	40
14.	2,4-Hexadien-1-ol	98	C6H10O	38
15.	Cyclohexanone	98	C6H10O	38
16.	4H-1,2,4-Triazol-3-amine, 4-methyl-	98	C3H6N4	37
17.	1H-1,2,4-Triazol-3-amine, 5-methyl-	98	C3H6N4	32
18.	3-Octene, (Z)-	112	C8H16	27
19.	3-Octene, (E)-	112	C8H16	27
20.	2-Pentenal, 2-methyl-	98	C6H10O	25

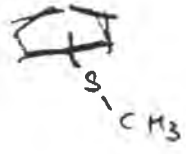
	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*78	000108-94-1	117743	60	29	1	99	9	46	0	39	9480
2.	*78	000108-94-1	819	53	37	0	73	9	46	11	40	9089
3.	*72	000108-94-1	117748	50	12	0	99	15	42	11	40	9442
4.	*59	029372-32-5	438	38	70	0	60	25	33	6	39	5967
5.	*56	000108-94-1	117749	51	42	1	99	12	30	6	35	9431
6.	*50	000592-78-9	901	32	60	3	193	18	25	0	33	9325
7.	*47	000108-94-1	117747	47	59	3	99	37	20	0	40	8322
8.	*45	003859-41-4	750	43	56	1	55	25	19	3	36	7258
9.	*43	000591-12-8	117674	33	55	0	73	43	18	0	41	9142
10.	*43	000108-94-1	117745	39	44	3	257	43	18	0	39	8961
11.	*40	006089-09-4	757	36	75	1	43	31	16	0	35	6033
12.	*40	000098-00-0	117681	32	83	0	63	31	16	0	33	6677
13.	*40	000098-00-0	117685	32	97	0	63	34	16	0	33	6050
14.	*38	000111-28-4	117760	33	63	2	107	48	14	0	39	8600
15.	*38	000108-94-1	117746	37	61	3	161	46	14	0	39	9036
16.	*37	016681-76-8	723	29	31	0	51	43	13	0	33	5926
17.	*32	004923-01-7	117660	31	33	0	63	46	9	0	33	5510
18.	*27	014850-22-7	2642	44	48	1	53	59	8	4	38	8838
19.	*27	014919-01-8	2643	34	58	1	57	56	8	13	40	8813
20.	*25	000623-36-9	117703	29	63	0	70	51	7	0	33	7859

Peak 126



Average of 7.448 to 7.481 min.: A1026.D
Converted from RTE data file: >A1026:
Modified:added subtracted scaled

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	192	110.00	745				
52.95	26	111.95	29				
58.95	74						
63.90	16						
67.00	112						
68.00	25						
82.90	156						
83.25	11						
84.90	69						
94.95	1577						
96.00	121						



C_6H_6S

or $C_6H_6O_2$

C_6	72
H	6.
S	32

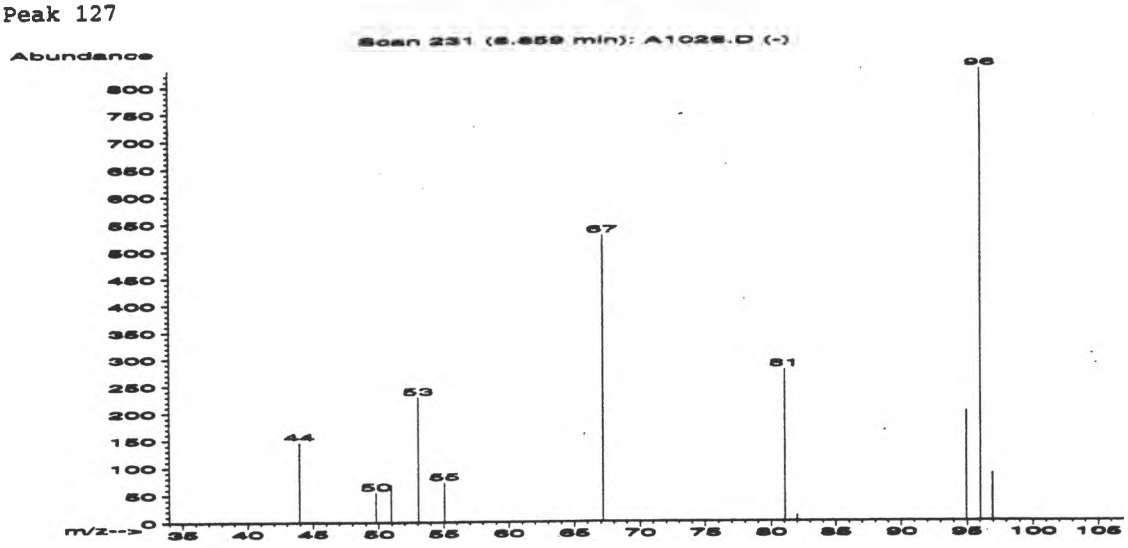
Average of 7.448 to 7.481 min.: A1026.D
Converted from RTE data file: >A1026:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(2-furanyl)-	110	C6H6O2	72
2.	Ethanone, 1-(2-furanyl)-	110	C6H6O2	56
3.	Ethanone, 1-(2-furanyl)-	110	C6H6O2	56
4.	Ethanone, 1-(2-furanyl)-	110	C6H6O2	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	001192-62-7	2127	33	44	1	82	14	42	0	41	9929
2.	*56	001192-62-7	118826	29	48	1	99	14	30	0	33	9922
3.	*56	001192-62-7	118828	32	47	1	99	14	30	0	33	9885
4.	*40	001192-62-7	118827	28	63	1	99	14	16	0	29	9897

Peak 127



Scan 231 (8.859 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.95	146						
49.80	54						
50.95	68						
53.05	229						
55.05	72						
67.15	525						
81.05	278						
82.00	10						
94.95	201						
96.05	830						
96.95	86						

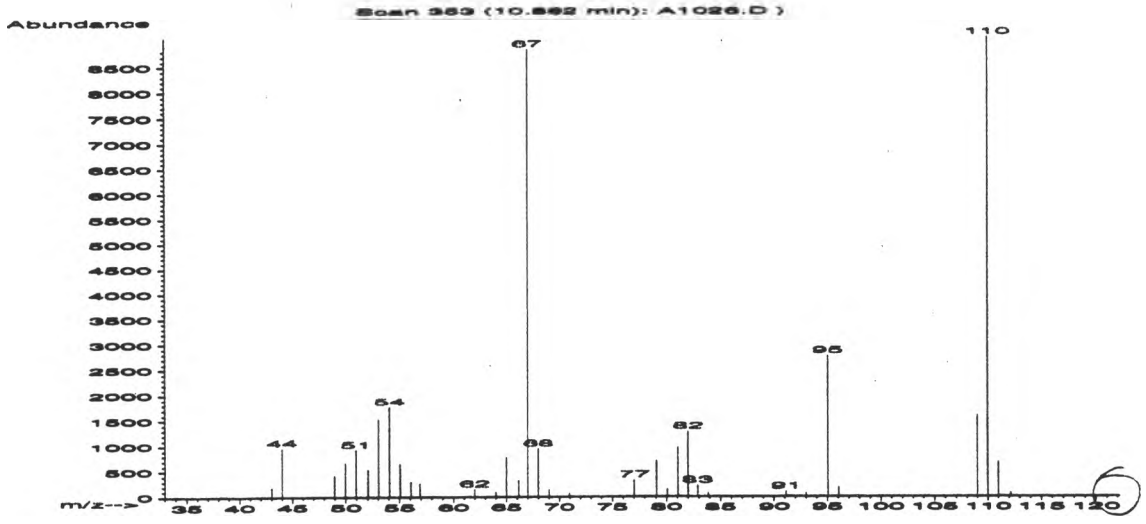
Scan 231 (8.859 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	86
2.	Furan, 2,5-dimethyl-	96	C6H8O	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	002758-18-1	594	51	53	1	84	10	53	0	44	9791
2.	*40	000625-86-5	117589	38	53	1	76	35	16	0	33	8055

Peak 17a (Peak 17 in original contains impurity)



Scan 353 (10.862 min): A1026.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	188	62.00	151	81.05	969	112.15	83
44.00	962	64.00	87	82.00	1278		
48.95	419	65.00	773	82.90	218		
49.95	672	66.15	326	83.90	70		
50.95	924	67.00	8825	91.15	97		
52.05	542	68.00	946	93.00	59		
53.05	1533	69.00	140	95.05	2765		
54.05	1769	70.95	69	96.05	185		
55.05	651	77.05	329	109.00	1597		
56.05	298	79.05	698	110.00	9066		
56.90	268	80.05	149	111.00	678		

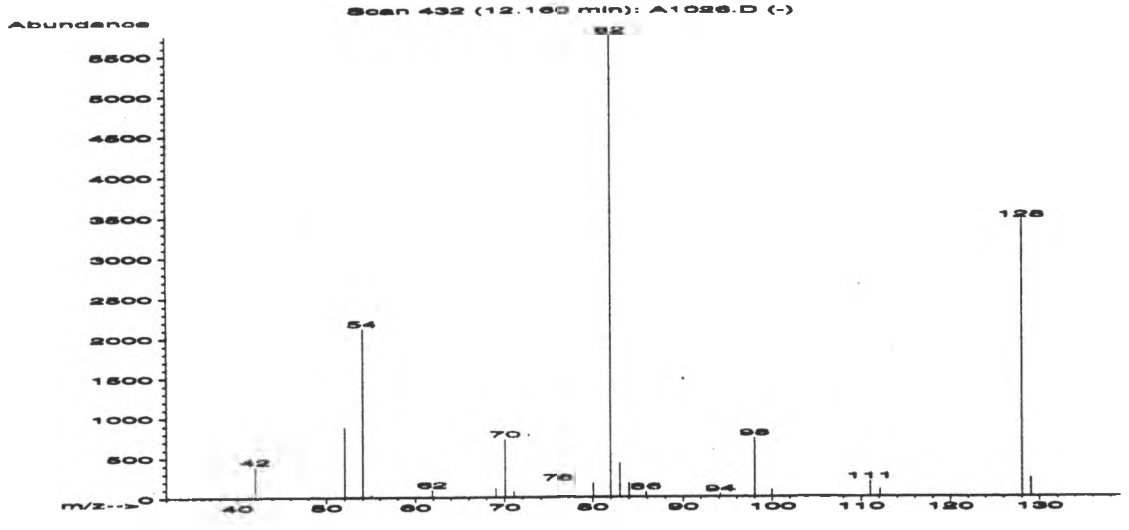
Scan 353 (10.862 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-Cyclohexen-1-al	110	C7H10O	80
2.	2,3-DIMETHYL-2-CYCLOPENTEN-1-ONE	110	C7H10O	80
3.	Spiro[2.4]heptan-4-one	110	C7H10O	53
4.	3-Octyne	110	C8H14	52
5.	Cyclopropane, 1,2-dimethyl-3-methylene-	82	C6H10	50
6.	Cyclopentane, methylene-	82	C6H10	38
7.	Cyclopentene, 1-methyl-	82	C6H10	38
8.	1H-Imidazole-2-carboxaldehyde, 1-methyl-	110	C5H6N2O	38
9.	p-Benzoquinone, compd. with resorcinol (	218	C12H10O4	38
10.	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	38
11.	Cyclopentene, 3-methyl-	82	C6H10	35
12.	2,4-Hexadiene	82	C6H10	35
13.	1-Hexyne	82	C6H10	35
14.	4(1H)-Pyrimidinone, 6-methyl-	110	C5H6N2O	35
15.	1,3-Benzenediol	110	C6H6O2	35
16.	1,4-Benzenediol	110	C6H6O2	35
17.	Cyclopropane, (1-methylethenyl)-	82	C6H10	30
18.	1,3-Benzenediol	110	C6H6O2	30
19.	Cyclopropane, (1-methylethenyl)-	82	C6H10	27
20.	1,4-Benzenediol	110	C6H6O2	27

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	001192-88-7	2182	35	8	0	93	12	48	16	43	6065
2.	*80	001121-05-7	2188	57	43	1	95	12	48	0	49	9794
3.	*53	005771-32-4	2199	40	64	3	87	26	28	20	38	9011
4.	*52	015232-76-5	118878	50	53	3	75	33	27	23	45	8660
5.	*50	062338-02-7	116779	65	28	0	72	50	25	0	64	6877
6.	*38	001528-30-9	116785	28	50	0	69	50	14	22	42	6807
7.	*38	000693-89-0	116781	44	31	0	97	54	14	18	47	6823
8.	*38	013750-81-7	118817	44	44	2	94	54	14	17	47	6880
9.	38	026734-94-1	42712	38	72	3	91	49	14	14	39	7129
10.	*38	001072-91-9	118843	47	50	2	79	48	14	0	40	6871
11.	*35	001120-62-3	116783	29	43	0	97	54	11	20	42	6790
12.	*35	000592-46-1	116772	57	23	0	74	52	11	2	38	6504
13.	35	000693-02-7	116757	46	34	0	88	52	11	2	41	6825
14.	*35	003524-87-6	2115	37	55	3	84	52	11	0	39	7256
15.	*35	000108-46-3	2130	35	53	2	98	54	11	5	40	7025
16.	*35	000123-31-9	118840	33	53	1	70	55	11	1	40	7048
17.	*30	004663-22-3	116778	36	41	0	68	56	9	11	43	6860
18.	*30	000108-46-3	118836	37	14	0	90	58	9	10	43	6927
19.	*27	004663-22-3	116777	40	58	0	70	56	8	0	39	6843
20.	*27	000123-31-9	2131	38	49	2	79	58	8	0	39	7063

Peak 128



Scan 432 (12.160 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
42.00	381	82.00	5747				
52.05	873	83.00	426				
54.05	2109	84.00	174				
55.00	25	85.90	66				
61.90	94	94.15	36				
69.00	111	98.05	736				
70.05	723	99.95	85				
71.05	69	111.00	189				
75.95	180	112.10	89				
78.00	56	128.05	3435				
80.05	174	129.05	234				

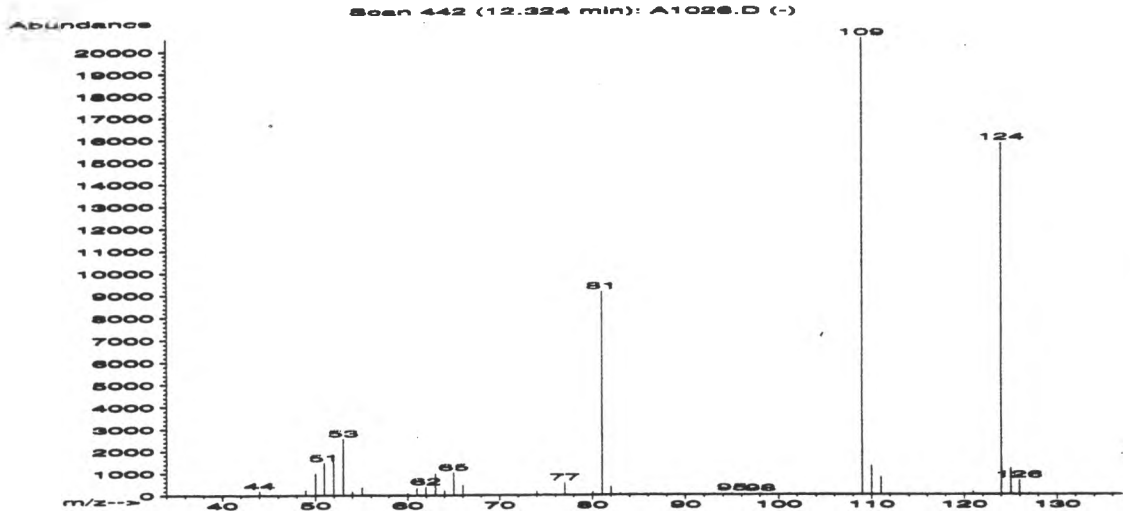
Scan 432 (12.160 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Nitrobenzene-d5	123	C6D5NO2	91
2.	Nitrobenzene-d5	123	C6D5NO2	83
3.	1-METHYL-2,4,5-TRIOXOIMIDAZOLIDINE	128	C4H4N2O3	10
4.	1-METHYL-2,4,5-TRIOXOIMIDAZOLIDINE	128	C4H4N2O3	10
5.	1H-Azepine, hexahydro-1-nitroso-	128	C6H12N2O	10
6.	1,3-DIMETHYL-4-AMINO-1,2,4-TRIAZOLE-5-ON	128	C4H8N4O	8

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*91	000000-00-0	120299	73	19	1	79	2	60	24	59	9745
2.	*83	000000-00-0	4529	60	37	1	85	13	50	0	56	9867
3.	*10	003659-97-0	120729	32	71	0	57	68	1	0	33	4504
4.	*10	003659-97-0	5675	28	71	0	57	69	1	0	33	4453
5.	*10	000932-83-2	120768	30	72	1	76	63	1	0	29	5006
6.	* 8	004114-16-3	5679	28	68	1	59	68	1	0	26	4916

Peak 129



Scan 442 (12.324 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
44.00	205	61.95	394	83.00	63	125.05	1186
48.95	236	63.00	985	84.00	14	125.95	628
50.00	977	64.00	233	93.05	32	127.00	40
50.95	1453	65.00	1021	95.00	71		
51.95	1672	66.00	461	98.05	47		
53.00	2540	74.00	183	109.00	20562		
54.00	155	75.05	34	110.00	1295		
55.05	355	77.00	544	111.00	779		
56.00	7	80.05	139	112.00	27		
60.00	77	81.05	9117	120.95	128		
61.00	328	82.00	371	124.05	15794		

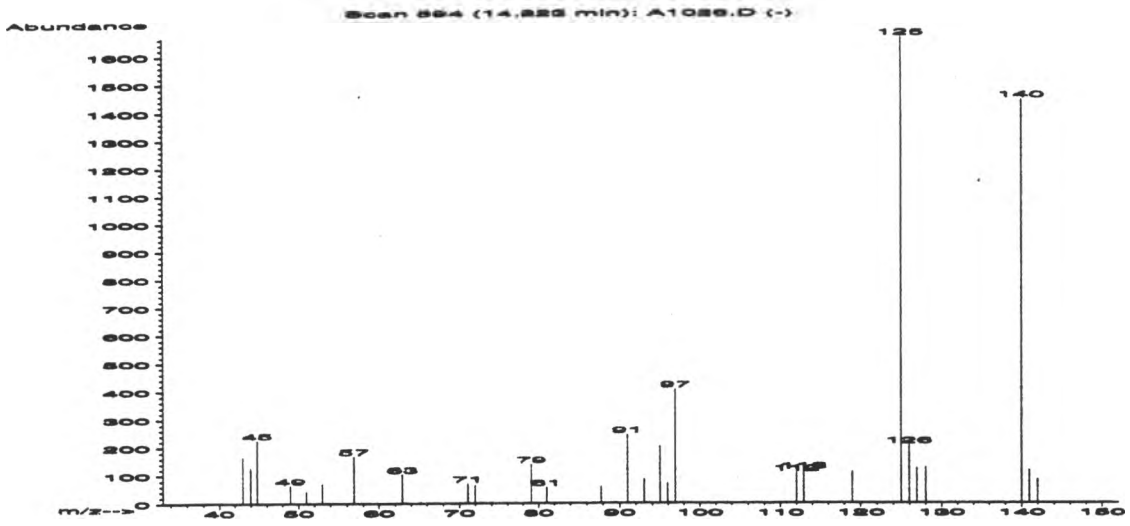
Scan 442 (12.324 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2-methoxy-	124	C7H8O2	90
2.	Phenol, 2-methoxy-	124	C7H8O2	90
3.	Phenol, 2-methoxy-	124	C7H8O2	86
4.	2-Acetyl-5-methylfuran	124	C7H8O2	80
5.	2-Cyclopenten-1-one, 3,4,5-trimethyl-	124	C8H12O	78
6.	Phenol, 4-methoxy-	124	C7H8O2	78
7.	Phenol, 2-methoxy-	124	C7H8O2	78
8.	Phenol, 4-methoxy-	124	C7H8O2	64
9.	2-Cyclopenten-1-one, 2,3,4-trimethyl-	124	C8H12O	59
10.	Phenol, 2-methoxy-	124	C7H8O2	58
11.	METHYL-(5(4)-METHYLIMIDAZOL-4(5)-YL)KETO	124	C6H8N2O	56
12.	2-Cyclopenten-1-one, 3,4,4-trimethyl-	124	C8H12O	50
13.	Phenol, 3-amino-	109	C6H7NO	38
14.	Phenol, 2-methoxy-	124	C7H8O2	32
15.	2,3-Pyridinediamine	109	C5H7N3	32
16.	Phenol, 2-amino-	109	C6H7NO	32
17.	Phenol, 2-methoxy-	124	C7H8O2	23
18.	Pyridine, 2-methyl-, 1-oxide	109	C6H7NO	17
19.	Benzene, (fluoromethyl)-	110	C7H7F	12
20.	3-FLUOROCYCLOHEPTATRIENE	110	C7H7F	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*90	000090-05-1	120383	79	9	1	87	6	59	35	74	9818
2.	*90	000090-05-1	120377	75	15	2	81	6	59	0	81	9965
3.	*86	000090-05-1	120379	65	24	2	90	6	53	0	47	9983
4.	*80	001193-79-9	4688	33	39	0	88	13	48	14	43	9195
5.	*78	055683-21-1	4786	41	47	3	76	8	46	17	39	9812
6.	*78	000150-76-5	120385	58	26	1	68	6	46	2	41	9972
7.	*78	000090-05-1	120376	59	29	1	73	6	46	9	40	9872
8.	*64	000150-76-5	120386	53	39	2	70	9	37	0	35	9933
9.	*59	028790-86-5	4783	34	66	2	63	25	33	0	41	9868
10.	*58	000090-05-1	120382	36	52	2	61	28	32	8	43	9874
11.	*56	023328-91-8	4661	30	33	0	97	11	30	0	33	9628
12.	*50	030434-65-2	120405	37	48	2	99	16	25	15	37	9434
13.	*38	000591-27-5	2058	45	43	1	79	46	14	0	40	7933
14.	32	000090-05-1	4705	41	45	0	63	46	9	6	35	9970
15.	*32	000452-58-4	2030	32	51	1	92	48	9	0	33	7957
16.	*32	000095-55-6	2057	42	48	1	69	49	9	0	35	7653
17.	*23	000090-05-1	120378	32	52	2	67	48	6	4	29	7328
18.	*17	000931-19-1	2040	30	72	2	81	53	3	0	27	7400
19.	12	000350-50-5	118849	39	45	1	84	58	2	0	28	6615
20.	12	000000-00-0	2156	33	53	1	70	56	2	0	21	7041

Peak 130



Scan 594 (14.823 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	165	79.05	137	112.90	115		
43.95	127	81.05	55	119.00	111		
44.80	224	83.00	1	124.95	1665		
48.95	63	85.95	1	125.95	204		
50.95	40	87.75	58	126.95	125		
53.00	69	91.00	243	128.00	127		
56.90	166	93.00	86	140.00	1443		
62.90	102	94.95	201	141.00	117		
65.20	5	95.95	71	142.00	84		
71.05	68	96.95	404				
71.95	64	112.00	106				

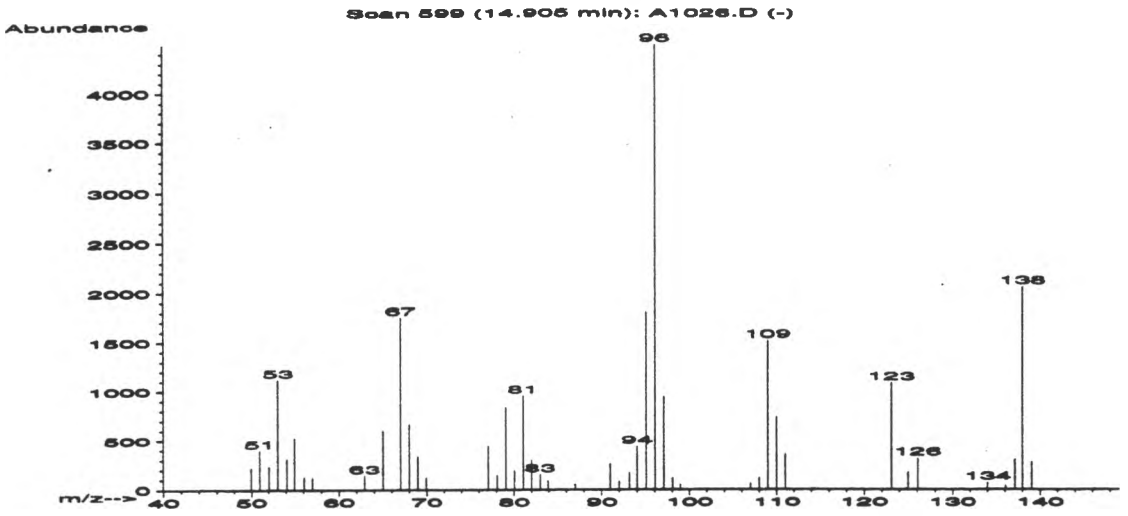
Scan 594 (14.823 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 4-(methylthio)-	140	C7H8OS	80
2.	Phenol, 4-(methylthio)-	140	C7H8OS	80
3.	1H-Pyrazole, 1-(trimethylsilyl)-	140	C6H12N2Si	64
4.	Benzene, (methylsulfinyl)-	140	C7H8OS	53
5.	Benzene, (methylsulfinyl)-	140	C7H8OS	53
6.	Phenol, 2-(methylthio)-	140	C7H8OS	49
7.	Phenol, 2-(methylthio)-	140	C7H8OS	49
8.	2-ACETYL-3-METHYLTHIOPHENE	140	C7H8OS	47
9.	2-Butenal, diethylhydrazone	140	C8H16N2	39
10.	METHYLESTER OF 2-METHYLENE-3-HEXENE CARB	140	C8H12O2	39
11.	Benzenethiol, 2-amino-	125	C6H7NS	38
12.	2(1H)-Pyridinethione, 4-methyl-	125	C6H7NS	35
13.	Thiophene, 3-(1,1-dimethylethyl)-	140	C8H12S	28
14.	Thiophene, 2-(1,1-dimethylethyl)-	140	C8H12S	28
15.	Acetonitrile, (4-oxo-2-thiazolidinyliden	140	C5H4N2OS	27
16.	2(1H)-Pyridinethione, 5-methyl-	125	C6H7NS	23
17.	Benzenethiol, 2-amino-	125	C6H7NS	23
18.	2(1H)-Pyridinone, 4-hydroxy-6-methyl-	125	C6H7NO2	23
19.	2-AMINO-6-METHYL-4-PYRIMIDINOL	125	C5H7N3O	23
20.	Thiophene, 3-(1,1-dimethylethyl)-	140	C8H12S	17

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*80	001073-72-9	122414	56	43	1	79	11	48	5	49	9810
2.	*80	001073-72-9	9093	55	49	1	77	13	48	0	49	9893
3.	*64	018156-75-7	9067	44	39	1	97	20	37	16	38	9190
4.	*53	001193-82-4	9090	41	54	0	66	29	28	5	38	9871
5.	*53	001193-82-4	122412	47	48	0	74	27	28	18	39	9869
6.	*49	001073-29-6	122413	49	48	0	68	38	23	0	46	8875
7.	*49	001073-29-6	9092	49	51	0	67	40	23	0	46	8837
8.	47	000000-00-0	9087	53	42	0	80	36	20	0	39	9446
9.	*39	025186-07-6	9284	32	88	1	74	20	15	0	26	9811
10.	*39	072707-70-1	9173	30	30	1	99	18	15	0	27	9677
11.	*38	000137-07-5	120453	34	77	1	93	47	14	0	39	7508
12.	*35	018368-65-5	4969	34	70	0	68	54	11	0	41	7483
13.	28	001689-79-8	122458	36	58	3	81	38	8	0	22	8930
14.	28	001689-78-7	9275	35	58	2	92	38	8	0	22	8839
15.	*27	003364-82-7	9014	34	78	0	64	59	8	0	41	6586
16.	*23	018368-58-6	4970	31	81	1	99	47	6	0	29	7520
17.	*23	000137-07-5	120454	28	60	1	99	47	6	0	29	7509
18.	*23	003749-51-7	120451	29	68	1	93	48	6	0	27	7501
19.	*23	000000-00-0	4946	28	78	1	98	50	6	0	27	7497
20.	*17	001689-79-8	122459	31	49	1	126	54	3	7	29	8930

Peak 48a



Scan 599 (14.905 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
49.95	221	68.00	662	87.00	56	108.00	116
50.95	398	69.00	334	91.00	258	109.00	1509
52.05	232	69.95	121	92.00	83	110.00	734
53.05	1116	77.05	443	93.15	172	111.00	356
54.05	311	78.05	147	94.00	436	123.05	1079
54.95	524	79.05	832	95.05	1798	124.95	170
56.05	128	80.05	191	96.05	4489	126.05	315
57.00	117	81.05	949	97.05	939	134.00	67
62.90	138	82.00	299	98.05	113	136.05	38
65.00	597	83.00	152	98.95	50	137.15	301
67.00	1745	83.95	91	107.00	60	138.00	2047

Scan 599 (14.905 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
139.00	277						

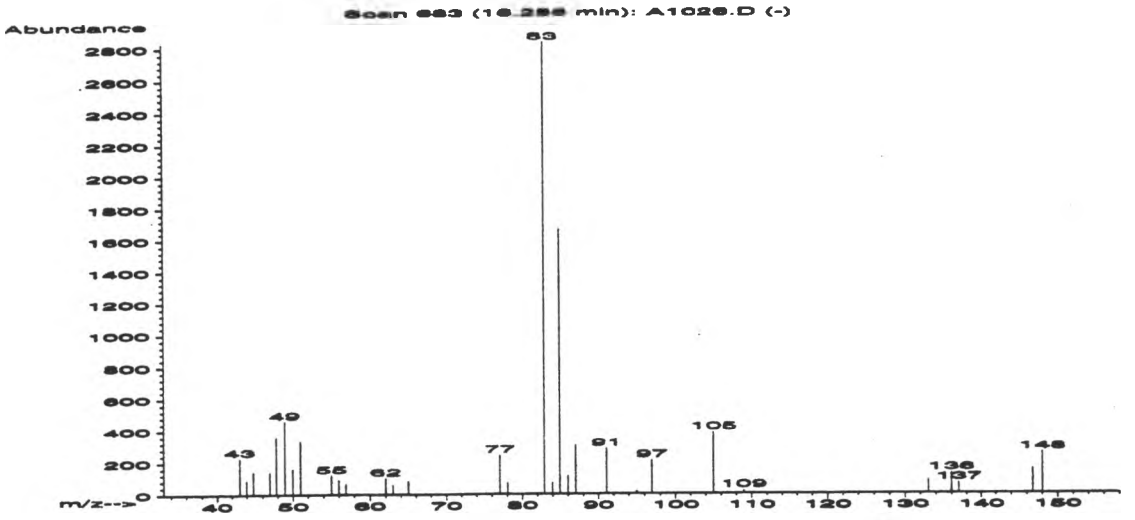
Scan 599 (14.905 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	2-Cyclohexen-1-one, 4,4,5-trimethyl-	138	C9H14O	49
2.	2-Cyclohexen-1-one, 3,4,4-trimethyl-	138	C9H14O	47
3.	2,4-Hexadienal	96	C6H8O	47
4.	2-Cyclohexen-1-one, 4,4,6-trimethyl-	138	C9H14O	46
5.	2-Propanone, 1-cyclohexylidene-	138	C9H14O	46
6.	Spiro[4.5]decane	138	C10H18	38
7.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	37
8.	2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	37
9.	2H-Pyran-2-one, 4,6-dimethyl-	124	C7H8O2	37
10.	Cyclohexanone, hydrazone	112	C6H12N2	32
11.	1H-Indene, octahydro-	124	C9H16	32
12.	5-Methyl-6-ethyl-2-pyrone	138	C8H10O2	27
13.	4,N'-DIMETHYL HISTAMINE	139	C7H13N3	25
14.	Bicyclo[3.3.1]non-3-en-2-ol, exo-	138	C9H14O	25
15.	Pyridine, 1,2,5,6-tetrahydro-1,2-dimethy	111	C7H13N	22
16.	N-1,5,7-TRIMETHYL-2,3-DIHYDRO-1,4-DIAZEP	139	C8H15N2	22
17.	CIS-DIMETHYL-ISOPROPYLIDENE CYCLOPROPANE	110	C8H14	18
18.	1,2-Benzisoxazole, octahydro-, (3aR-cis)	127	C7H13NO	14
19.	1-(2-Furyl)-butan-3-one	138	C8H10O2	12
20.	1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*49	017429-29-7	8623	36	65	2	87	39	23	10	43	9299
2.	*47	017299-41-1	122267	45	65	2	81	36	20	0	39	8868
3.	*47	000142-83-6	575	40	49	0	96	38	20	11	40	8043
4.	*46	013395-73-8	8624	61	45	2	130	43	20	0	46	9406
5.	*46	000874-68-0	8640	55	56	0	71	45	20	0	49	6172
6.	*38	000176-63-6	8822	52	59	2	64	40	14	10	35	9148
7.	*37	002758-18-1	117591	45	49	2	99	43	13	3	30	8483
8.	*37	002758-18-1	594	33	50	1	99	45	13	12	35	8348
9.	37	000675-09-2	4695	45	53	0	99	41	13	15	37	8197
10.	32	006156-08-7	2508	43	66	3	121	46	9	0	37	8389
11.	32	000496-10-6	4933	39	69	3	99	48	9	9	31	8706
12.	*27	062968-85-8	8499	43	35	2	239	56	8	0	40	5620
13.	*25	053966-46-4	8921	29	70	1	95	52	7	0	33	8236
14.	*25	010060-21-6	8684	33	85	2	51	51	7	6	37	9452
15.	*22	015031-95-5	2370	41	45	0	73	62	5	6	39	8030
16.	*22	000000-00-0	8960	44	79	2	95	63	5	0	40	5419
17.	*18	000000-00-0	2261	37	47	0	31	67	3	14	43	4952
18.	14	064018-30-0	5612	43	50	2	33	68	2	16	38	4557
19.	*12	000000-00-0	8483	35	68	1	65	61	2	0	35	6018
20.	*10	000694-48-4	559	36	55	1	79	69	1	9	32	7947

Peak 131



Scan 683 (16.286 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	228	62.00	101	91.10	283		
43.95	89	63.00	60	95.00	17		
44.80	138	65.00	82	96.95	209		
46.95	138	77.05	243	105.05	381		
47.80	358	78.05	71	108.95	20		
48.95	459	81.95	1	133.00	81		
49.95	160	82.90	2831	136.00	126		
50.95	333	83.95	70	137.00	65		
55.05	119	84.90	1662	146.80	152		
55.95	91	86.00	113	148.05	254		
56.90	65	87.00	305				

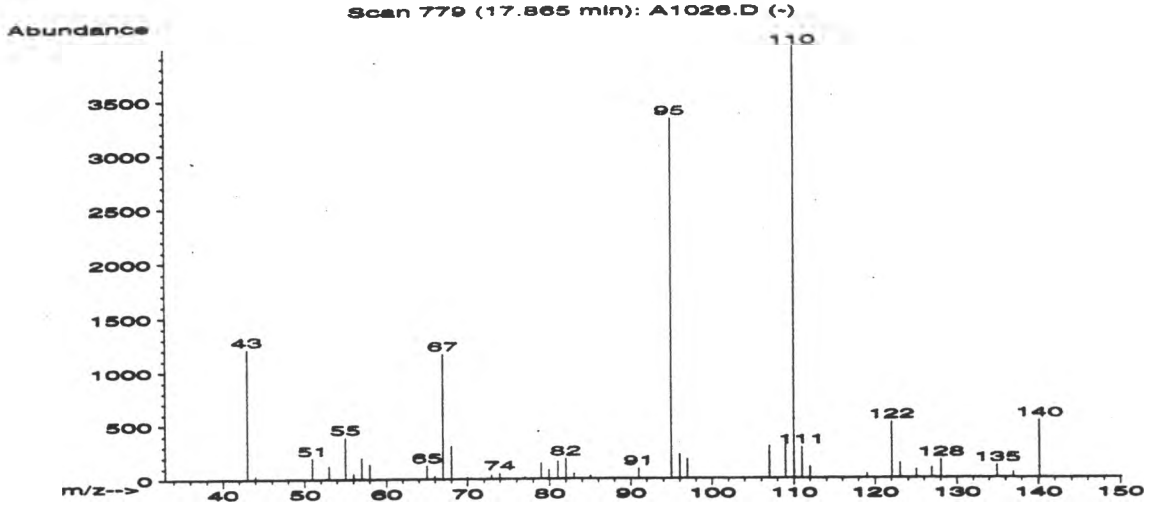
Scan 683 (16.286 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Acetyl chloride, dichloro-	146	C2HCl3O	72
2.	Methane, oxybis[dichloro-	182	C2H2Cl4O	50
3.	Hexanoic acid, 2-methyl-3-oxo-, ethyl es	172	C9H16O3	50
4.	Chloroform	118	CHCl3	50
5.	TETRANEURIN - C -	366	C19H26O7	39
6.	Ethane, 1,1-dichloro-2,2-difluoro-	134	C2H2Cl2F2	39
7.	Acetic acid, trichloro-	162	C2HCl3O2	39
8.	Chloroform	118	CHCl3	39
9.	Chloroform	118	CHCl3	39
10.	Chloroform	118	CHCl3	39
11.	Methane, bromodichloro-	162	CHBrCl2	39
12.	Methane, bromodichloro-	162	CHBrCl2	39
13.	Pyrrolidine, 1-[8-(3-octyloxiranyl)-1-ox	351	C22H41NO2	39
14.	Ethane, 1,1,2-trichloro-	132	C2H3Cl3	39
15.	Methane, bromodichloro-	162	CHBrCl2	38
16.	Isothiazole	85	C3H3NS	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*72	000079-36-7	11103	50	51	1	82	15	42	19	40	9521
2.	50	020524-86-1	26203	48	73	2	89	16	25	0	31	9722
3.	50	029304-40-3	126133	42	59	3	88	16	25	0	33	9739
4.	50	000067-66-3	119702	47	59	1	74	16	25	0	35	9547
5.	39	028587-46-4	91537	33	113	2	84	19	15	0	20	9794
6.	39	000471-43-2	7179	40	69	1	87	16	15	0	28	9806
7.	39	000076-03-9	125014	34	36	1	78	16	15	0	21	9535
8.	39	000067-66-3	119704	34	45	2	88	19	15	2	22	9666
9.	39	000067-66-3	119703	48	56	1	66	16	15	0	27	9585
10.	39	000067-66-3	3697	48	56	1	66	16	15	0	27	9585
11.	39	000075-27-4	125009	33	54	1	90	19	15	1	23	9791
12.	39	000075-27-4	17356	33	59	1	92	19	15	2	23	9742
13.	39	056630-37-6	134973	42	98	2	91	16	15	2	22	9459
14.	39	000079-00-5	121296	42	95	1	91	16	15	0	28	9860
15.	38	000075-27-4	125010	35	43	1	90	22	14	0	21	9680
16.	* 9	000288-16-4	116935	28	38	1	58	76	1	0	33	4941

Peak 132



Scan 779 (17.865 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1212	68.00	308	85.00	28	122.05	522
44.00	32	69.15	7	91.00	95	123.05	137
50.95	194	70.05	16	94.95	3321	125.05	80
53.00	123	72.95	37	96.00	223	126.95	97
55.00	389	73.95	55	96.95	177	128.05	167
56.00	52	77.00	20	107.00	301	135.00	117
57.00	199	79.00	147	109.00	384	136.95	49
58.00	138	79.95	89	110.00	3990	140.15	534
65.00	125	81.00	161	111.00	290		
65.95	32	82.00	187	112.00	108		
67.00	1163	83.00	53	119.00	40		

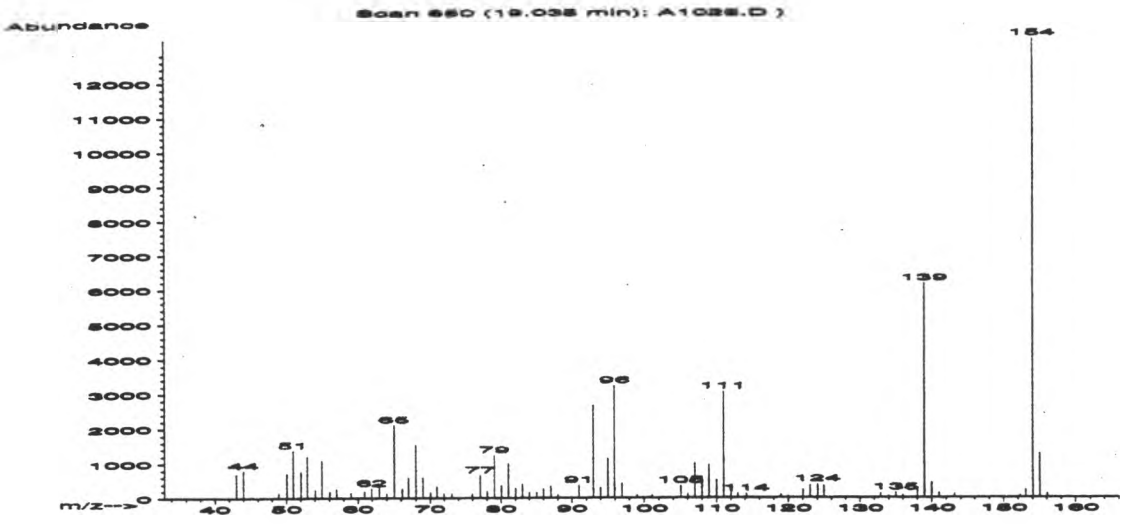
Scan 779 (17.865 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	MENTHENE ISOMER B	138	C10H18	72
2.	2-PENTANOYLFURAN	152	C9H12O2	42
3.	2-HEXANOYL FURAN	166	C10H14O2	36
4.	2-HEPTANOYL FURAN	180	C11H16O2	36
5.	2-HEXANOYL FURAN	166	C10H14O2	36
6.	CYCLOHEXENE, 1,3-DIMETHYL-	110	C8H14	32
7.	1H-Imidazole-2-carboxaldehyde, 1-methyl-	110	C5H6N2O	27
8.	1H-Imidazole-4-ethanamine, .beta.-methyl	125	C6H11N3	22
9.	2-Decyne	138	C10H18	17
10.	Ethanone, 1-bicyclo[2.2.1]hept-2-yl-, ex	138	C9H14O	17
11.	2-(1',1'-DIDEUTERO-N-BUTYL)PYRIDINE	135	C9H11D2N	17
12.	Cyclohexaneethanol	128	C8H16O	17
13.	1,4-Pentadiene, 2,3,4-trimethyl-	110	C8H14	17
14.	Bicyclo[2.2.1]heptane-2-carboxaldehyde,	124	C8H12O	16
15.	BICYCLO[2.2.1]HEPTANE, 2-FORMYL-	124	C8H12O	16
16.	2(1H)-Pyridinone	95	C5H5NO	16
17.	2(1H)-Pyridinone	95	C5H5NO	16
18.	Phenol, 2-ethoxy-	138	C8H10O2	12
19.	2,3-Dimethyl-3-isopropyl-cyclopentene	138	C10H18	12
20.	Cyclohexene, 1-methyl-3-(1-methylethyl)-	138	C10H18	12

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	72	029350-67-2	122308	57	25	1	79	15	42	1	38	9785
2.	42	000000-00-0	123920	41	26	1	92	26	17	2	31	9700
3.	36	000000-00-0	125558	40	25	1	85	26	12	0	29	9631
4.	36	000000-00-0	25596	33	49	2	99	27	12	0	25	9634
5.	36	000000-00-0	19378	33	45	1	90	27	12	0	22	9628
6.	32	000000-00-0	2280	44	48	1	67	50	9	0	35	7943
7.	*27	013750-81-7	118817	36	54	2	71	58	8	0	39	7429
8.	*22	024160-35-8	4987	34	52	0	59	64	5	0	41	6184
9.	17	002384-70-5	8717	35	75	3	55	53	3	0	22	6646
10.	17	000824-59-9	8660	37	54	1	68	53	3	0	20	6527
11.	17	000000-00-0	7593	39	57	2	55	52	3	0	29	6285
12.	17	004442-79-9	6023	34	64	1	55	51	3	0	22	7721
13.	17	072014-90-5	118897	37	46	2	69	55	3	0	22	6667
14.	16	003574-55-8	4822	43	47	1	55	56	3	0	35	6439
15.	16	000000-00-0	4827	43	47	1	55	56	3	0	35	6439
16.	*16	000142-08-5	117539	31	23	1	83	56	3	1	30	6503
17.	*16	000142-08-5	520	32	43	0	65	56	3	2	35	6508
18.	12	000094-71-3	122226	35	60	1	67	58	2	0	22	7431
19.	12	073331-73-4	8770	37	38	1	62	60	2	0	25	6315
20.	12	013828-31-4	8790	34	53	2	82	58	2	0	21	6354

Peak 133



Scan 850 (19.035 min): A1026.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	694	59.00	162	70.95	329	84.00	169
44.00	793	60.90	199	71.95	139	85.00	171
48.95	150	61.90	286	73.05	125	86.00	261
50.05	709	63.00	388	75.95	116	87.00	350
50.95	1378	64.00	133	77.05	658	88.00	93
52.05	766	65.00	2102	78.05	203	91.00	370
52.95	1208	66.15	277	79.05	1232	93.00	2683
54.05	247	67.00	585	80.05	358	94.00	291
54.95	1097	68.00	1537	81.05	1005	95.05	1140
56.05	190	69.00	588	82.00	294	95.95	3228
57.00	276	70.05	166	83.00	402	96.95	422

Scan 850 (19.035 min): A1026.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
99.05	91	114.15	126	138.00	237		
101.05	85	119.00	105	139.00	6156		
105.05	360	119.95	51	140.00	446		
106.05	113	122.05	234	141.00	147		
107.00	1003	123.05	368	143.15	102		
108.00	610	124.05	397	152.30	71		
109.00	957	124.95	346	153.05	224		
110.00	516	132.90	125	154.05	13248		
111.00	3054	134.00	48	155.05	1271		
112.00	258	135.00	150	156.05	122		
113.00	130	136.00	77				

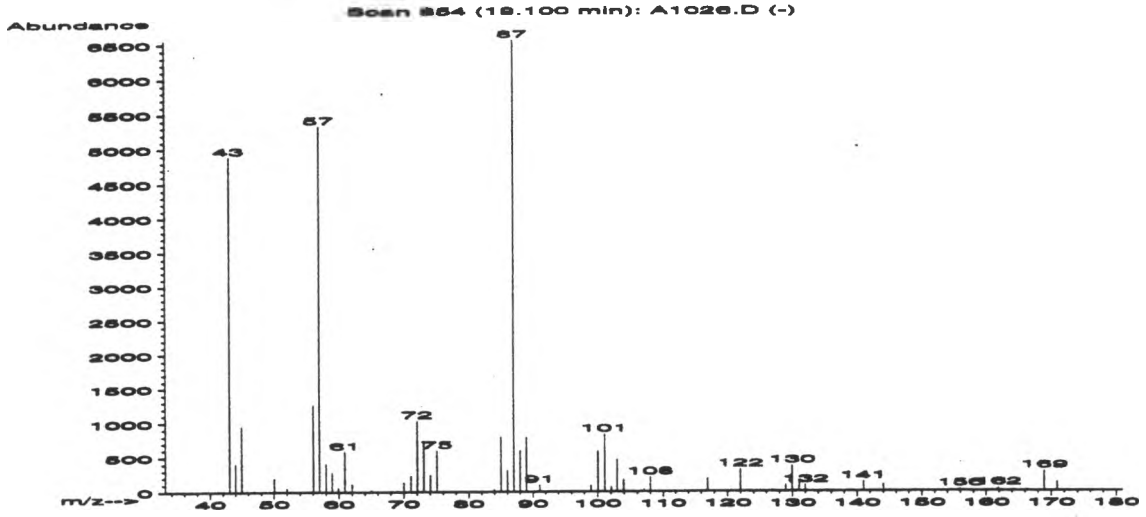
Scan 850 (19.035 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Phenol, 2,6-dimethoxy-	154	C8H10O3	94
2.	Phenol, 2,6-dimethoxy-	154	C8H10O3	91
3.	Phenol, 2,6-dimethoxy-	154	C8H10O3	58
4.	1,3-Cyclohexanedione, 2,5,5-trimethyl-	154	C9H14O2	50
5.	Phenol, 3,4-dimethoxy-	154	C8H10O3	47
6.	Phenol, 3,4-dimethoxy-	154	C8H10O3	45
7.	Benzene, 1-methoxy-2-(methylthio)-	154	C8H10OS	42
8.	1,3-Dimethyl-melamine	154	C5H10N6	42
9.	Phenol, 3-methyl-4-(methylthio)-	154	C8H10OS	40
10.	Phenol, 3,4-dimethoxy-	154	C8H10O3	38
11.	Benzoic acid, 3,5-dihydroxy-	154	C7H6O4	38
12.	1-METHOXY-4-FLUOROFORMYL-BENZENE	154	C8H7FO2	37
13.	Methylphloroglucinol-.beta.-monomethylet	154	C8H10O3	32
14.	Benzene, 1-methoxy-3-(methylthio)-	154	C8H10OS	32
15.	1,3-Dimethyl-melamine	154	C5H10N6	28
16.	L-Alanine, N-methyl-N-(trifluoroacetyl)-	255	C10H16F3NO3	25
17.	Alanine, 2-methyl-N-(trifluoroacetyl)-,	255	C10H16F3NO3	25
18.	Benzoic acid, 3,4-dihydroxy-	154	C7H6O4	25
19.	Benzoic acid, 3,5-dihydroxy-	154	C7H6O4	25
20.	2,3-DIAMINO-5-NITROPYRIDINE	154	C5H6N4O2	23

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*94	000091-10-1	14321	88	18	1	76	0	70	0	89	9971
2.	*91	000091-10-1	124139	85	13	0	83	4	62	41	80	9476
3.	*58	000091-10-1	124140	57	44	1	74	26	32	0	49	9914
4.	*50	001125-11-7	14448	35	45	2	92	33	25	0	39	9512
5.	*47	002033-89-8	124141	65	40	1	68	40	20	0	41	9471
6.	*45	002033-89-8	124142	56	40	2	85	21	19	8	32	9637
7.	*42	002388-73-0	14296	39	59	3	96	26	17	2	31	9667
8.	*42	000000-00-0	124111	42	34	3	99	28	17	11	37	9379
9.	*40	003120-74-9	14295	43	44	2	78	34	16	13	36	9389
10.	*38	002033-89-8	14322	50	45	2	99	38	14	1	34	9140
11.	*38	000099-10-5	14233	49	51	2	67	54	14	0	44	8301
12.	*37	000000-00-0	14279	42	66	2	83	42	13	0	33	8925
13.	*32	055382-24-6	14320	30	54	2	93	47	9	0	33	9225
14.	*32	002388-74-1	14297	24	68	3	99	47	9	2	32	9106
15.	*28	000000-00-0	14201	29	43	1	99	38	8	0	27	9333
16.	25	034815-08-2	131515	45	68	3	72	55	7	0	37	8428
17.	25	034815-07-1	58400	39	83	3	88	55	7	0	33	8533
18.	*25	000099-50-3	124121	37	60	2	93	52	7	0	35	8482
19.	*25	000099-10-5	124122	40	55	2	99	52	7	0	33	8463
20.	*23	000000-00-0	14192	29	90	3	99	47	6	0	29	8719

Peak 134



Scan 854 (19.100 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4889	62.00	106	83.95	33	102.95	459
44.00	411	65.00	21	85.00	798	103.95	176
44.95	949	66.00	6	86.00	311	107.00	26
50.05	194	68.00	5	87.00	6557	108.00	209
52.00	53	69.10	14	88.00	598	117.00	178
56.05	1260	70.00	135	89.00	788	121.95	318
57.00	5331	71.05	228	91.05	100	128.95	86
58.00	411	72.05	1027	99.00	87	129.95	369
58.95	283	73.05	735	100.05	586	131.05	126
59.90	59	74.05	238	101.05	835	132.00	88
60.90	582	75.05	597	102.05	67	141.00	140

Scan 854 (19.100 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
144.05	96						
155.95	30						
161.90	40						
168.95	291						
170.95	125						

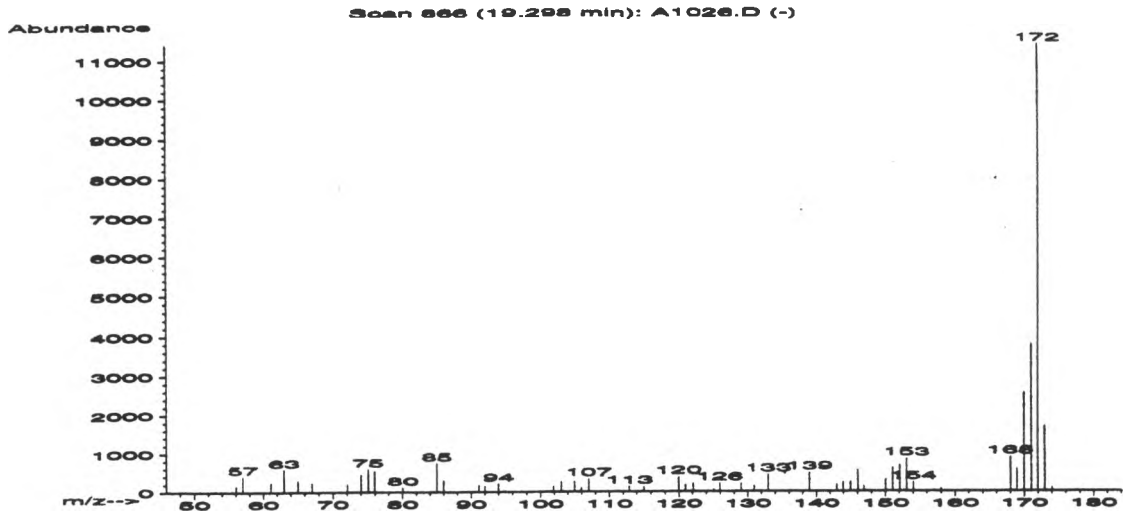
Scan 854 (19.100 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanol, 2-(2-butoxyethoxy)-, acetate	204	C10H20O4	90
2.	Ethanol, 2-(2-butoxyethoxy)-, acetate	204	C10H20O4	64
3.	Cyclobutene, 3,4-dichloro-	122	C4H4Cl2	47
4.	1,3-Dioxolane-2-ethanol, 2-methyl-	132	C6H12O3	43
5.	Acetamide, N-ethyl-	87	C4H9NO	43
6.	Methanol, dibutoxy-	176	C9H20O3	40
7.	.alpha.-D-Xylofuranoside, methyl 3-O-met	178	C7H14O5	38
8.	3,4-DI-O-METHYL-L-ARABINOPYRANOSE	178	C7H14O5	38
9.	2-O-METHYL-D-MANNOPYRANOSA	194	C7H14O6	38
10.	6,8-DIOXABICYCLO(3.2.1)OCTAN-2L-OL	130	C6H10O3	38
11.	3-HYDROXYISOBUTYRIC ACID ISOPROPYL ESTER	146	C7H14O3	38
12.	Ethane, isothiocyanato-	87	C3H5NS	38
13.	D-Fructose, 3-O-methyl-	194	C7H14O6	38
14.	1,3-Butadiene, 1,4-dichloro-	122	C4H4Cl2	37
15.	MONOETHYL ESTER OF MALONIC ACID	132	C5H8O4	25
16.	Butane, 1,1'-oxybis-	130	C8H18O	25
17.	Ethanol, 2,2'-[1,2-ethanediylbis(oxy)]bi	234	C10H18O6	25
18.	2-N-BUTOXYETHYL GLYCIDYL ETHER	174	C9H18O3	12
19.	2-Butanone, 1-(acetyloxy)-	130	C6H10O3	11
20.	Butyl glycol acetate	160	C8H16O3	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	90	000124-17-4	36294	109	7	0	75	2	57	4	46	9978
2.	64	000124-17-4	128610	77	33	0	68	18	37	4	39	9695
3.	*47	041326-64-1	120118	44	36	1	98	40	20	16	38	7498
4.	43	005754-32-5	121350	47	36	2	99	43	18	17	38	7787
5.	*43	000625-50-3	130	33	59	2	107	45	18	0	41	7594
6.	40	054518-04-6	23756	39	49	2	142	35	16	0	33	9307
7.	38	034338-86-8	24439	51	49	3	76	37	14	5	33	7642
8.	38	086049-20-9	24446	45	58	3	93	37	14	0	37	7648
9.	38	036864-61-6	31489	42	56	2	89	40	14	14	35	7590
10.	*38	000000-00-0	6338	34	76	2	86	39	14	0	35	9696
11.	38	000000-00-0	11272	43	70	2	99	37	14	0	37	7624
12.	*38	000542-85-8	117134	34	61	1	99	48	14	0	39	7581
13.	38	036256-85-6	31483	55	60	3	81	40	14	0	36	7592
14.	*37	002984-42-1	4274	38	42	1	92	43	13	9	30	7510
15.	*25	000000-00-0	6795	33	65	1	73	51	7	0	35	7500
16.	*25	000142-96-1	6583	31	55	2	387	45	7	0	29	7687
17.	25	000111-21-7	49711	39	54	0	89	52	7	12	37	7533
18.	12	013483-47-1	22960	52	41	0	57	62	2	0	35	7216
19.	*11	001575-57-1	6309	36	41	0	71	74	2	2	43	6307
20.	9	000112-07-2	16742	46	48	1	80	71	1	0	34	7995

Peak 59a



Scan 866 (19.298 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
56.05	153	80.05	114	112.90	132	143.00	160
57.00	401	85.00	746	115.00	111	143.95	233
61.15	236	86.00	293	119.95	378	144.95	235
63.00	577	91.15	171	120.95	152	146.05	548
65.00	298	92.00	145	122.05	199	146.95	119
67.00	226	94.00	202	125.05	48	150.05	296
72.05	194	101.95	128	125.95	214	151.05	599
73.00	9	103.05	257	129.05	200	152.05	676
74.05	454	104.95	253	130.95	135	153.05	840
75.05	589	105.95	96	132.95	440	154.05	228
75.95	539	107.00	329	139.00	485	157.00	19

Scan 866 (19.298 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
158.00	70						
168.00	885						
168.95	574						
169.95	2530						
171.05	3765						
171.95	11398						
172.95	1686						
174.05	87						

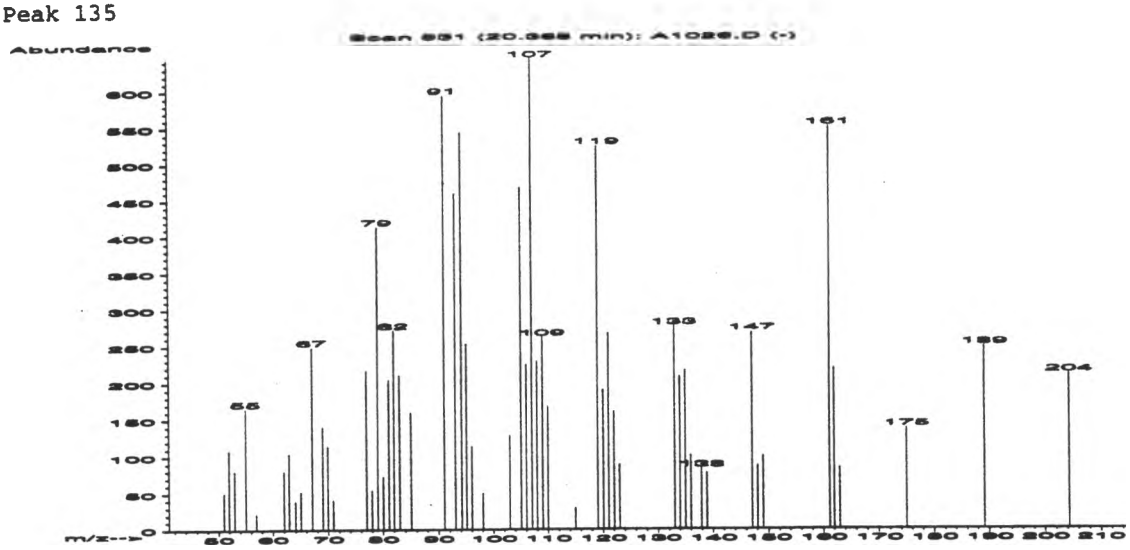
Scan 866 (19.298 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1,1'-Biphenyl, 2-fluoro-	172	C12H9F	81
2.	1,1'-Biphenyl, 4-fluoro-	172	C12H9F	74
3.	2,2'-Dipyridyl-oxide	172	C10H8N2O	50
4.	1-METHYL-4-METHOXYNAPHTHALENE	172	C12H12O	47
5.	2-(2-HYDROXYPHENYL)PYRIMIDINE	172	C10H8N2O	43
6.	Benzofuran, 3-methyl-2-(1-methylethenyl)	172	C12H12O	40
7.	2,2'-BITHIAZOLINE-2	172	C6H8N2S2	36
8.	4-(4-HYDROXYPHENYL)PYRIMIDINE	172	C10H8N2O	28
9.	2-Naphthalenecarboxylic acid	172	C11H8O2	25
10.	2-Naphthalenecarboxylic acid	172	C11H8O2	25
11.	2-Naphthalenecarboxylic acid	172	C11H8O2	25

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*81	000321-60-8	22421	77	21	1	66	17	49	26	66	9755
2.	*74	000324-74-3	22422	68	27	2	68	17	44	2	58	9735
3.	*50	000000-00-0	22257	35	82	2	89	31	25	0	41	9683
4.	*47	000000-00-0	22446	34	82	2	72	40	20	0	39	9421
5.	*43	064435-20-7	22264	40	55	3	97	42	18	0	39	9288
6.	*40	023911-58-2	22431	31	82	3	98	31	16	0	33	9655
7.	*36	000000-00-0	21966	29	96	2	99	29	12	0	29	9656
8.	*28	023380-78-1	22266	29	93	1	87	37	8	0	29	9366
9.	*25	000093-09-4	126215	28	85	3	99	43	7	0	29	9214
10.	*25	000093-09-4	126214	28	80	3	87	42	7	0	27	9249
11.	*25	000093-09-4	126213	28	83	3	97	43	7	0	27	9214

Peak 135



Scan 931 (20.368 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
50.95	51	69.95	114	93.05	458	110.00	167
51.95	108	70.95	40	94.15	542	115.00	29
52.95	80	77.00	216	95.05	252	119.05	524
55.00	165	78.00	54	96.05	113	120.05	190
56.95	22	79.05	413	98.05	50	121.05	267
62.00	80	80.05	72	102.95	128	122.05	161
62.90	104	81.05	204	105.05	466	123.05	88
64.00	39	82.00	271	106.05	224	133.00	276
65.00	52	83.00	210	107.00	644	134.00	208
67.05	248	85.00	159	108.00	228	135.00	216
69.00	140	91.05	593	109.00	261	136.00	101

Scan 931 (20.368 min): A1026.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
137.90	82						
138.90	77						
147.05	268						
148.05	87						
149.05	100						
161.15	550						
162.00	219						
163.00	84						
174.95	137						
189.15	248						
204.30	210						

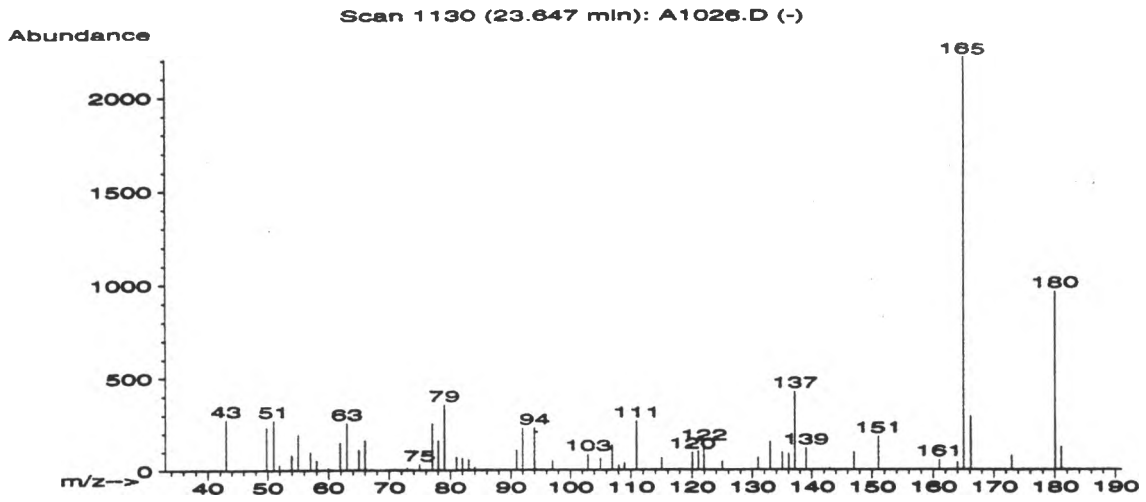
Scan 931 (20.368 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Junipene	204	C15H24	83
2.	Cyclopropa[d]naphthalen-2(4aH)-one, 1,1a	204	C14H20O	64
3.	(+)-Aromadendrene	204	C15H24	47
4.	Calarene	204	C15H24	38
5.	TRICYCLO[4.1.0.0(3,5)]HEPTANE, 2-ISOBUTE	204	C15H24	38
6.	Tricyclo[4.1.0.0(2,4)]heptane, 3,3,7,7-t	204	C15H24	38
7.	1,4,4,7a-Tetramethyl-5,6,7,7a-tetrahydro	176	C13H20	27
8.	Tricyclo[2.2.1.0(2,6)]heptane, 1,7-dimet	204	C15H24	27
9.	Calarene	204	C15H24	25
10.	Calarene	204	C15H24	18
11.	.gamma.-Cadinene	204	C15H24	15
12.	Tricyclo[2.2.1.0(2,6)]heptane, 1,7-dimet	204	C15H24	14
13.	Ethanone, 1-(3-methylphenyl)-	134	C9H10O	11
14.	ORTHO-D2-.GAMMA.-PHENYLPROPANOL	136	C9H10D2O	11
15.	.alpha.-Humulene	204	C15H24	11
16.	LIMONYL ALCOHOL	154	C10H18O	10
17.	2H-1-Benzopyran, 3,4-dihydro-2,2-dimethy	162	C11H14O	10
18.	Cyclohexane, 1,2-dimethyl-3,5-bis(1-meth	192	C14H24	10
19.	Tetracyclo[5.2.1.0(2,6).0(3,5)]decane, 4	162	C12H18	10
20.	CYCLOHEXANE,2A,3E-DIMETHYL-1E,5A-DIVINYL	164	C12H20	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	000475-20-7	128709	87	64	1	150	32	50	0	91	9725
2.	*64	004677-90-1	36609	78	79	2	147	46	37	0	84	9277
3.	*47	000489-39-4	128755	59	92	3	158	39	20	0	41	9443
4.	*38	017334-55-3	128758	75	76	1	145	46	14	1	41	6531
5.	38	000000-00-0	36784	56	96	0	70	50	14	1	40	7815
6.	38	056348-21-1	36783	56	96	0	70	50	14	1	40	7815
7.	27	051595-84-7	24065	53	38	0	93	57	8	18	39	6450
8.	27	000512-61-8	128748	62	85	2	214	57	8	0	39	7793
9.	*25	017334-55-3	36778	53	85	3	236	64	7	0	49	6805
10.	*18	017334-55-3	128759	55	85	1	166	67	3	0	47	7018
11.	*15	039029-41-9	128720	58	79	1	183	76	2	0	51	6469
12.	*14	000512-61-8	36766	56	97	0	61	67	2	1	40	7138
13.	*11	000585-74-0	121576	50	54	1	78	78	2	0	46	4135
14.	*11	053973-99-2	7949	44	71	0	61	79	2	0	44	6338
15.	*11	006753-98-6	36673	50	85	3	224	71	2	0	46	8290
16.	10	000000-00-0	14667	59	69	0	64	75	1	0	43	6176
17.	*10	001198-96-5	125160	33	69	0	78	78	1	0	41	5455
18.	10	062337-99-9	31106	75	57	0	75	75	1	12	39	6402
19.	*10	074646-38-1	17921	68	63	1	84	73	1	21	42	6406
20.	10	068779-12-4	18731	69	61	0	65	80	1	0	42	6703

Peak 136



Scan 1130 (23.647 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	274	65.00	110	91.00	108	115.00	66
49.80	233	66.00	161	92.00	229	120.05	96
50.95	270	72.95	14	94.00	229	121.05	102
51.90	28	75.00	32	95.95	3	121.95	143
53.95	82	77.05	254	97.00	51	125.00	47
55.00	194	78.05	162	102.95	85	130.95	66
57.00	98	79.05	356	105.05	63	133.00	153
58.00	53	81.05	73	107.00	136	135.00	95
59.95	12	82.00	65	108.05	26	136.10	88
61.90	149	83.00	56	109.00	39	137.15	425
63.00	255	84.00	17	111.00	265	139.00	119

Scan 1130 (23.647 min): A1026.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
143.00	10						
147.05	95						
151.05	183						
161.00	54						
164.00	43						
165.00	2210						
166.15	292						
172.95	78						
180.05	958						
181.05	123						

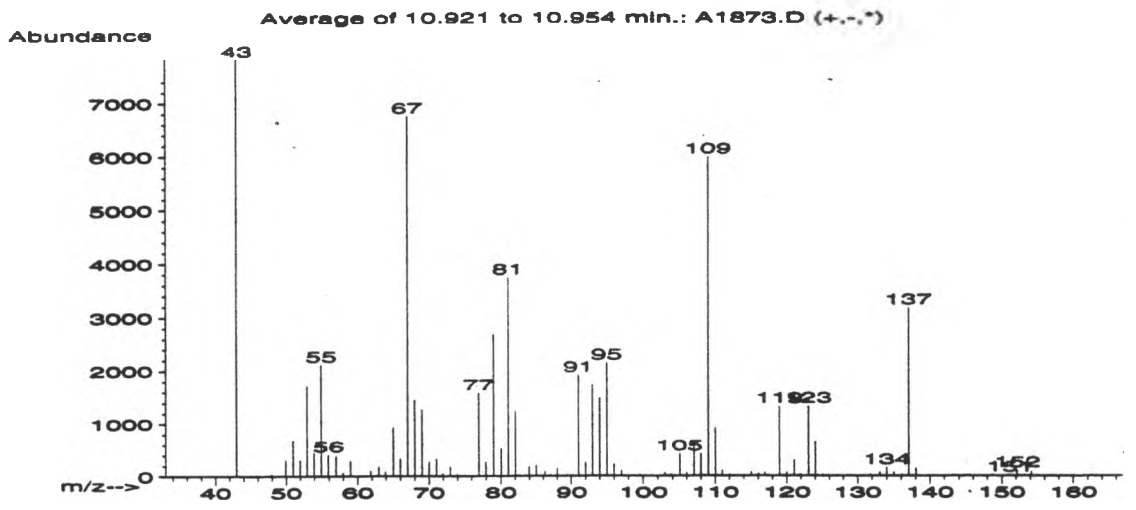
Scan 1130 (23.647 min): A1026.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	86
2.	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	80
3.	9-HYDROXY-1-METHYL-1,2,3,4-TETRAHYDRO-8H	180	C9H12N2O2	78
4.	4-METHOXY-3-METHYL-2,3-DIHYDROBENZOFURAN	180	C10H12O3	72
5.	TERTIO BUTYL HYDROXY ANISOLE	180	C11H16O2	64
6.	TERTIO BUTYL HYDROXY ANISOLE	180	C11H16O2	64
7.	3-TERT-BUTYL-4-METHOXYPHENOL	180	C11H16O2	64
8.	2,4-DIMETHOXY-ACETOPHENONE	180	C10H12O3	64
9.	Ethanone, 1-(2,5-dimethoxyphenyl)-	180	C10H12O3	59
10.	Benzenamine, N-ethyl-2-methyl-5-nitro-	180	C9H12N2O2	58
11.	Ethanone, 1-(2-hydroxy-5-methoxy-4-methy	180	C10H12O3	53
12.	Silane, trimethyl(3-methylphenoxy)-	180	C10H16OSi	53
13.	9H-Fluorene, 2-methyl-	180	C14H12	53
14.	2-Hydroxy-3-methoxy-4-methylacetophenone	180	C10H12O3	53
15.	TERT-BUTYL-2-METHOXY PHENOL	180	C11H16O2	53
16.	3-TERT-BUTYL-4-METHOXYPHENOL	180	C11H16O2	46
17.	Thiazolo[5,4-d]pyrimidine, 5-(ethylamino	180	C7H8N4S	45
18.	Phenol, (1,1-dimethylethyl)-4-methoxy-	180	C11H16O2	43
19.	Phenol, (1,1-dimethylethyl)-4-methoxy-	180	C11H16O2	43
20.	2,3,4,5,6,7-HEXAHYDRO-2,2,3-TRIMETHYL-4-	180	C11H16O2	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	001131-62-0	25522	65	40	2	99	10	53	1	47	9827
2.	*80	001131-62-0	126822	63	39	1	93	12	48	12	47	9819
3.	*78	065628-74-2	25433	41	8	0	99	6	46	0	39	9783
4.	*72	035616-63-8	25550	47	4	0	97	11	42	11	40	9710
5.	*64	000121-00-6	126833	46	44	0	79	20	37	14	43	9605
6.	*64	000121-00-6	25603	41	43	0	71	20	37	10	39	9486
7.	*64	000088-32-4	126836	47	53	0	72	19	37	1	40	9688
8.	*64	000000-00-0	25527	49	57	2	99	23	37	0	44	9719
9.	*59	001201-38-3	25521	48	57	2	85	25	33	0	39	9812
10.	*58	056288-95-0	25429	36	52	0	82	30	32	3	43	9644
11.	*53	004223-84-1	25520	36	45	2	68	28	28	0	39	9670
12.	*53	017902-31-7	25583	45	40	1	71	30	28	11	38	9649
13.	*53	001430-97-3	126890	45	60	1	68	28	28	0	39	9513
14.	*53	077869-43-3	25526	43	60	1	74	26	28	19	39	9265
15.	*53	053894-31-8	25602	42	53	1	99	26	28	13	39	9718
16.	*46	000088-32-4	25604	34	46	0	56	41	20	14	43	9295
17.	*45	019835-21-3	25346	39	74	1	80	23	19	0	35	9799
18.	*43	025013-16-5	126834	44	53	0	59	41	18	7	40	9469
19.	*43	025013-16-5	126835	39	59	0	54	41	18	3	38	9456
20.	*38	000000-00-0	25644	34	70	2	65	39	14	11	36	9742

Peak 137



Average of 10.921 to 10.954 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	7844	59.00	288	71.05	326	82.05	1231
47.95	41	60.45	7	71.95	51	83.95	170
49.90	306	61.80	100	73.00	176	85.00	203
50.95	682	62.95	176	73.95	26	86.20	81
51.95	304	63.90	83	74.40	4	87.00	27
52.95	1715	65.00	925	75.00	20	88.00	140
53.95	452	66.00	331	77.00	1578	89.25	14
54.95	2113	67.00	6742	77.95	272	89.65	5
55.95	410	68.00	1441	79.00	2670	90.00	6
57.00	388	69.00	1262	80.05	522	91.00	1910
57.95	64	70.00	272	81.05	3726	92.00	261

Average of 10.921 to 10.954 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
93.00	1728	106.00	60	116.95	66	134.00	161
94.00	1478	107.05	607	119.00	1323	135.00	69
95.00	2140	108.00	424	120.00	69	136.05	20
96.00	219	109.05	5967	121.05	302	137.05	3165
97.05	99	110.05	910	121.95	29	138.05	145
99.00	11	111.00	109	123.10	1328	139.00	9
99.50	16	111.95	24	124.05	654	139.80	14
101.05	11	112.25	7	125.05	23	140.45	14
102.95	64	115.05	76	130.95	5	142.05	2
103.80	28	115.75	12	131.75	31	143.40	6
105.00	423	116.05	51	133.10	61	146.45	2

Average of 10.921 to 10.954 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
146.90	10						
148.90	13						
149.90	5						
150.90	7						
151.15	13						
152.15	103						
153.15	17						
154.15	76						
155.50	7						
156.80	6						

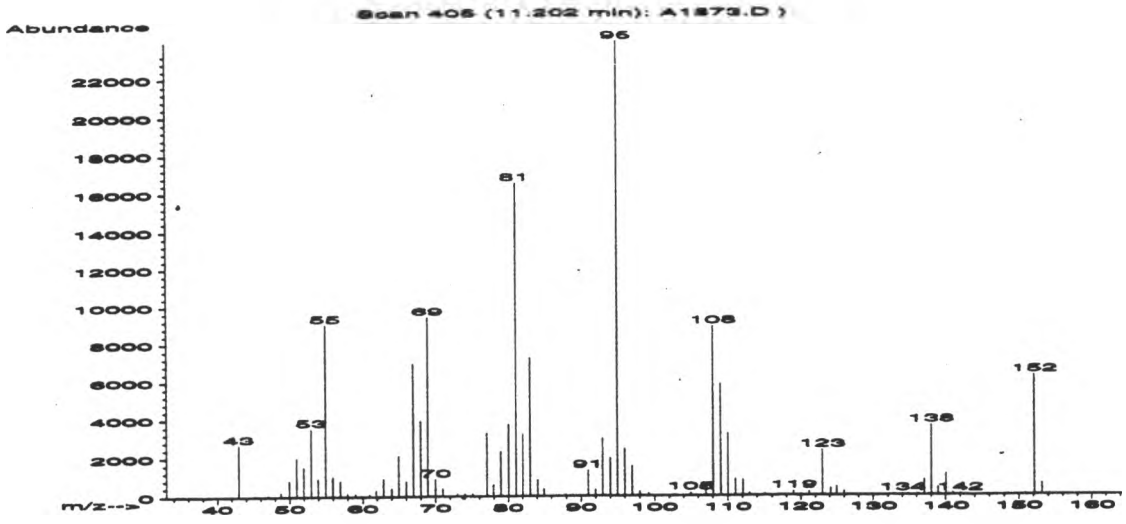
Average of 10.921 to 10.954 min.: A1873.D
Converted from RTE data file: >A1873:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	3-Octyne, 7-methyl-	124	C9H16	47
2.	trans-1-(2-Ethenylcyclohexyl)ethanone	152	C10H16O	47
3.	.beta.-Cyclocitral	152	C10H16O	45
4.	PHELLANDRAL	152	C10H16O	38
5.	Pyridine, 4-methoxy-	109	C6H7NO	27
6.	4-METHYLENE-5-HEXENAL	110	C7H10O	27
7.	4-Decyne	138	C10H18	22
8.	4-Nonyne	124	C9H16	22
9.	Cyclopentane, (1-methylethylidene)-	110	C8H14	22
10.	6,6-Dimethyl-2,3-diazabicyclo[3.1.0]hex-	110	C6H10N2	18
11.	4-Nonyne	124	C9H16	14
12.	1,3,7-Octatriene	108	C8H12	14
13.	1,3,7-Octatriene	108	C8H12	14
14.	Benzenemethanamine, 3-fluoro-	125	C7H8FN	14
15.	2(1H)-Pyridinone, 1-methyl-	109	C6H7NO	14
16.	4-Octyne	110	C8H14	11
17.	Cyclopropane, (1-methylethenyl)-	82	C6H10	10
18.	2,4-Hexadiene	82	C6H10	10
19.	Cyclopentene, 1-methyl-	82	C6H10	10
20.	1-(1,3-BUTADIENE-2-YL)-CYCLOPENTANOL	138	C9H14O	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	47	037050-06-9	120438	43	58	2	84	39	20	20	38	8845
2.	47	054678-07-8	13700	44	10	1	82	40	20	16	41	8649
3.	45	000432-25-7	13652	47	79	3	92	23	19	0	37	8554
4.	*38	023963-70-4	13650	62	47	1	51	50	14	6	38	8266
5.	*27	000620-08-6	2056	34	60	3	76	60	8	0	39	6556
6.	*27	000000-00-0	2163	50	53	2	62	60	8	18	39	6954
7.	*22	002384-86-3	8719	34	71	2	62	61	5	0	39	7944
8.	*22	020184-91-2	4865	47	51	1	85	64	5	0	40	7066
9.	*22	000765-83-3	2272	37	55	1	60	62	5	11	40	6697
10.	*18	068914-93-2	2146	53	53	2	70	68	3	0	47	6722
11.	*14	020184-91-2	120432	48	60	3	84	68	2	0	39	7255
12.	*14	001002-35-3	1942	37	53	1	78	68	2	0	39	6783
13.	*14	001002-35-3	118750	37	56	1	80	70	2	0	39	6687
14.	*14	000100-82-3	4993	40	41	1	72	69	2	0	39	5719
15.	*14	000694-85-9	118786	47	35	1	70	70	2	3	38	5683
16.	*11	001942-45-6	2219	36	47	0	41	78	2	25	43	6598
17.	*10	004663-22-3	116778	35	57	1	71	72	1	0	39	6464
18.	*10	000592-46-1	116772	49	32	1	82	73	1	19	39	6361
19.	*10	000693-89-0	116781	34	47	0	82	73	1	0	41	6361
20.	*10	000000-00-0	8613	35	79	1	28	75	1	5	40	8253

Peak 138



Scan 405 (11.202 min): A1873.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	2677	57.95	169	69.00	9429	82.05	3198
47.00	60	59.05	148	70.00	883	83.05	7261
48.80	209	59.80	39	71.00	370	84.05	829
49.95	819	60.95	109	73.00	120	84.95	355
50.95	1991	61.90	325	74.00	102	87.95	71
51.95	1514	62.90	911	75.05	125	88.90	71
52.95	3538	64.00	405	77.05	3299	91.00	1333
53.95	921	65.00	2115	77.95	599	92.00	316
54.95	9046	66.00	775	78.95	2330	93.00	2979
55.95	1036	67.00	6964	80.05	3751	94.00	1977
56.95	812	68.00	3917	81.05	16488	95.00	23928

Scan 405 (11.202 min): A1873.D

Modified:clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
96.00	2450	112.95	121	134.05	66	152.15	6298
97.00	1544	115.05	75	134.80	46	153.15	596
98.00	194	119.00	215	136.20	62	154.15	49
99.15	108	120.00	44	137.05	804		
104.95	168	121.15	178	138.05	3655		
107.05	517	123.00	2370	138.95	389		
108.05	8934	124.15	362	140.05	1106		
109.05	5874	125.00	449	141.05	112		
110.05	3234	126.00	214	142.05	58		
111.05	863	132.20	10	150.15	20		
112.05	819	132.95	20	150.90	42		

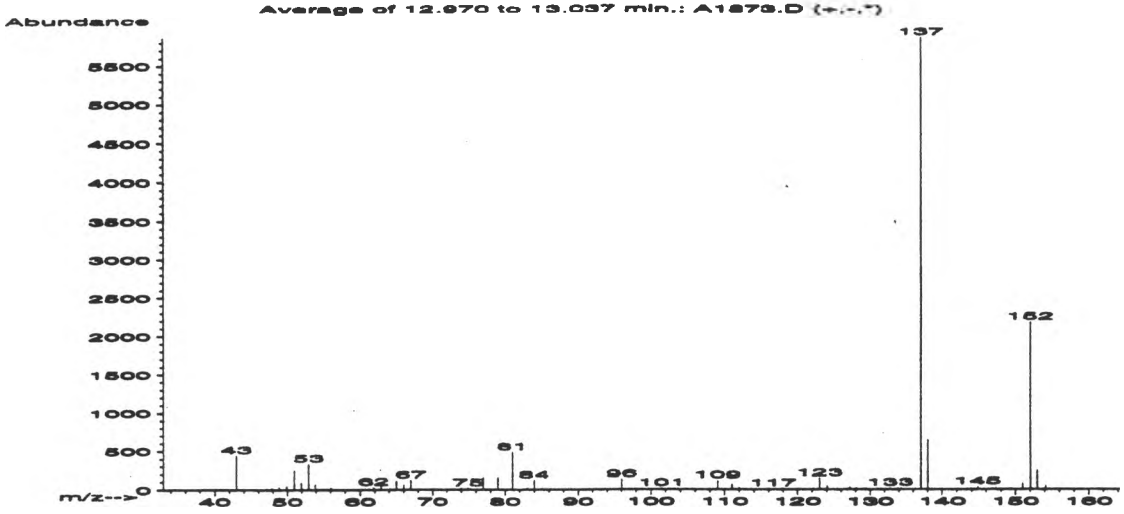
Scan 405 (11.202 min): A1873.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Camphor	152	C10H16O	96
2.	Camphor	152	C10H16O	95
3.	Camphor	152	C10H16O	95
4.	Camphor	152	C10H16O	94
5.	Camphor	152	C10H16O	94
6.	Camphor	152	C10H16O	94
7.	Camphor	152	C10H16O	93
8.	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimet	152	C10H16O	93
9.	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimet	152	C10H16O	90
10.	Camphor	152	C10H16O	83
11.	Camphor	152	C10H16O	81
12.	Camphor	152	C10H16O	70
13.	Bicyclo[3.1.0]hexan-2-one, 4-methyl-1-(1	152	C10H16O	46
14.	Cyclopentene, 1,4-dimethyl-5-(1-methylet	138	C10H18	43
15.	Cyclohexene, 1-methyl-3-(1-methylethyl)-	138	C10H18	43
16.	Cyclopentene, 1-isopropyl-2,3-dimethyl-	138	C10H18	41
17.	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	38
18.	Cyclohexene, 1-methyl-4-(1-methylethyl)-	138	C10H18	38
19.	Cyclohexene, 3-methyl-6-(1-methylethyl)-	138	C10H18	38
20.	Cyclohexene, 4-methyl-1-(1-methylethyl)-	138	C10H18	38

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*96	000076-22-2	13784	101	16	0	86	9	76	0	96	9874
2.	*95	000076-22-2	124020	99	12	0	82	9	74	56	95	9712
3.	*95	000076-22-2	124018	92	22	0	71	9	74	0	95	9811
4.	*94	000076-22-2	124022	98	16	0	70	9	70	57	94	9817
5.	*94	000076-22-2	124021	105	11	0	64	28	70	46	95	9714
6.	*94	000076-22-2	124019	105	11	0	64	28	70	46	95	9714
7.	*93	000076-22-2	124024	99	20	1	77	9	68	0	93	9836
8.	*93	000464-48-2	13786	106	12	1	82	9	66	46	91	9856
9.	*90	021368-68-3	13785	83	22	0	83	9	59	27	74	9852
10.	83	000076-22-2	124025	102	16	0	73	14	50	0	56	9809
11.	*81	000076-22-2	124017	85	40	1	79	19	49	0	80	9841
12.	*70	000076-22-2	124023	93	26	1	95	28	41	33	78	9794
13.	*46	002506-61-8	13714	57	57	1	44	45	20	0	47	8816
14.	*43	061142-33-4	8772	51	36	0	84	50	18	0	46	8485
15.	*43	013828-31-4	8790	51	37	0	95	50	18	0	46	8481
16.	*41	007712-73-4	8765	62	43	2	78	52	16	0	56	7956
17.	*38	000756-02-5	118896	51	40	1	89	51	14	0	46	8459
18.	*38	005502-88-5	8792	63	47	1	53	65	14	0	64	8469
19.	*38	005256-65-5	8795	54	55	2	98	54	14	0	47	8545
20.	*38	000500-00-5	122314	70	34	1	76	53	14	8	47	8497

Peak 139



Average of 12.970 to 13.037 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	440	60.25	6	76.95	154	101.95	2
47.15	9	61.20	11	79.00	153	102.45	3
47.65	6	61.90	28	81.00	481	103.70	6
47.90	20	62.90	68	83.00	15	109.05	112
48.85	32	64.15	10	84.00	119	111.00	64
49.90	45	65.00	103	85.00	13	112.00	19
50.95	247	66.00	58	89.00	3	113.00	1
51.95	86	67.00	118	96.00	131	116.00	7
52.95	330	73.75	6	100.75	8	116.30	1
53.90	73	74.00	17	101.15	8	116.65	9
56.00	23	74.95	17	101.45	12	117.95	4

Average of 12.970 to 13.037 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.15	11	132.75	15	151.00	71		
123.05	141	133.80	14	152.05	2168		
124.05	47	134.30	14	153.00	248		
127.20	27	137.05	5865	154.15	46		
128.10	15	138.05	638				
129.05	8	142.05	4				
129.25	4	143.95	9				
129.55	4	144.85	34				
130.55	2	146.85	11				
130.95	6	147.35	5				
131.45	6	149.40	5				

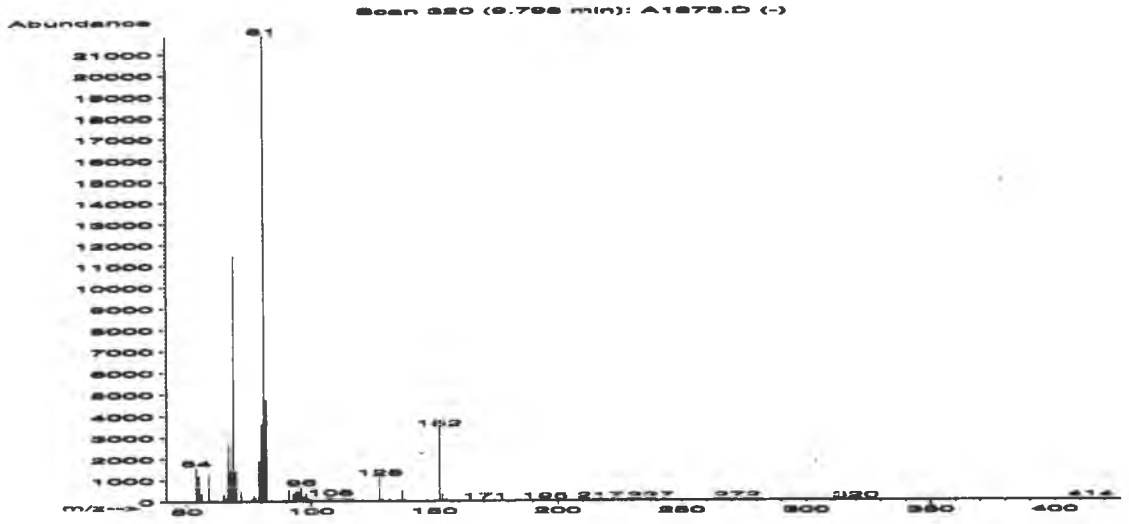
Average of 12.970 to 13.037 min.: A1873.D
Converted from RTE data file: >A1873:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Ethanone, 1-(2,4-dihydroxyphenyl)-	152	C8H8O3	86
2.	1-tert-Butyl-3,4-dimethylpyrazole	152	C9H16N2	78
3.	Pyrazine, 2-methoxy-3-(1-methylethyl)-	152	C8H12N2O	78
4.	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	78
5.	2-Methyl-1,3-benzoxathiole	152	C8H8OS	78
6.	2-ISOPROPYL-4-METHOXYPYRIMIDINE	152	C8H12N2O	74
7.	2,3-DIHYDROXY-ACETOPHENONE	152	C8H8O3	72
8.	Ethanone, 1-(2,4-dihydroxyphenyl)-	152	C8H8O3	64
9.	Phenol, 4-ethyl-2-methoxy-	152	C9H12O2	56
10.	Pyrazine, 2-methoxy-3-(1-methylethyl)-	152	C8H12N2O	56
11.	4(1H)-Pyrimidinone, 6-methyl-2-(1-methyl	152	C8H12N2O	56
12.	2-Methyl-1-(isopropylamino)-1-cyanobuten	152	C9H16N2	40
13.	4(1H)-Pyrimidinone, 6-methyl-2-(1-methyl	152	C8H12N2O	40
14.	1,3-DIAZIN, 6-HYDROXY-2-ISOPROPYL-4-METH	152	C8H12N2O	40

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*86	000089-84-9	13359	50	36	1	81	9	53	0	46	9977
2.	*78	063989-68-4	13551	31	10	0	99	9	46	9	42	9902
3.	*78	025773-40-4	13395	35	59	3	93	9	46	0	41	9976
4.	*78	002785-89-9	13455	39	39	1	98	7	46	9	42	9709
5.	*78	000000-00-0	13331	40	51	2	74	7	46	0	39	9949
6.	*74	064958-53-8	13387	28	16	0	99	2	44	0	33	9814
7.	*72	013494-10-5	13358	34	38	3	68	11	42	0	41	9880
8.	*64	000089-84-9	123904	41	43	3	70	9	37	5	35	9964
9.	*56	002785-89-9	123923	31	57	1	92	11	30	1	30	9975
10.	*56	025773-40-4	123917	31	43	1	73	11	30	1	30	8739
11.	*56	002814-20-2	123914	41	32	1	92	11	30	8	37	9884
12.	*40	066102-53-2	13548	31	79	2	99	11	16	0	29	9928
13.	*40	002814-20-2	13384	29	82	1	89	11	16	0	29	9841
14.	*40	000000-00-0	13399	29	82	1	89	11	16	0	29	9841

Peak 140



Scan 320 (9.798 min): A1873.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
53.95	1582	70.95	38	91.00	565	103.80	14
54.95	1192	72.00	492	91.95	22	104.90	38
55.95	373	76.00	103	93.00	367	105.90	41
59.05	1267	76.95	257	94.05	469	107.00	74
60.05	88	78.00	153	95.00	442	107.95	179
65.00	332	79.00	1901	96.00	653	114.30	63
66.00	151	80.05	3606	97.00	209	115.00	18
67.00	2658	81.00	21832	98.00	346	115.90	59
68.00	1469	82.05	4727	99.00	124	117.00	116
69.00	11474	84.00	44	99.90	77	118.75	36
70.00	1456	89.15	86	100.80	24	119.00	34

Scan 320 (9.798 min): A1873.D

Modified:subtracted

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
120.95	79	138.05	102	208.40	10		
122.00	7	138.80	36	217.05	19		
123.00	22	147.00	33	220.30	18		
128.00	1122	152.15	3409	237.40	16		
129.15	121	153.15	333	261.75	11		
130.45	22	154.15	74	269.80	12		
132.05	116	155.00	144	272.30	19		
135.05	43	160.20	29	319.80	10		
135.45	34	161.45	54	414.40	21		
136.05	60	170.65	5				
137.05	529	194.95	11				

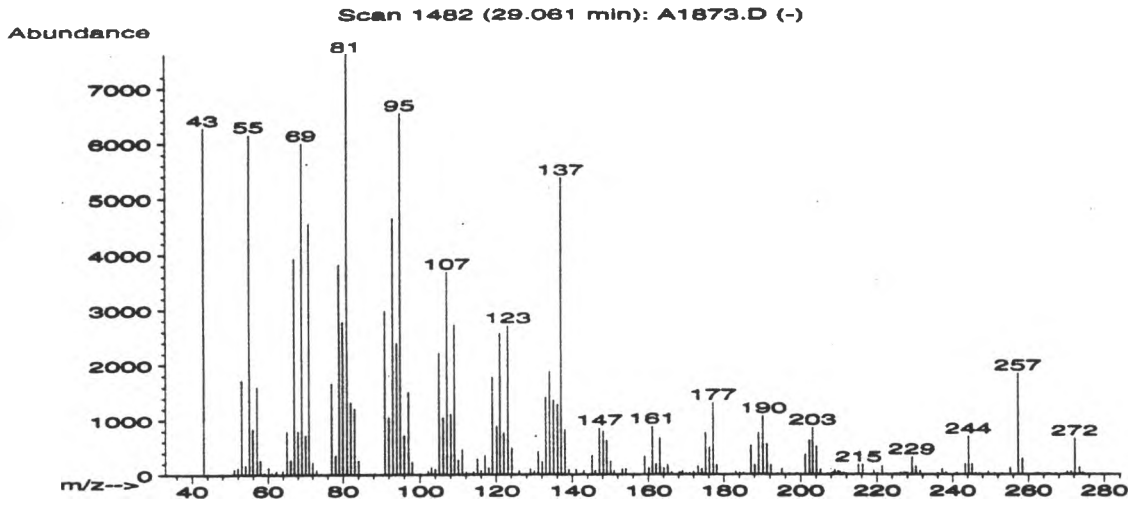
Scan 320 (9.798 min): A1873.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	Fenchone	152	C10H16O	83
2.	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimet	152	C10H16O	74
3.	Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimet	152	C10H16O	72
4.	Fenchone	152	C10H16O	64
5.	Fenchone	152	C10H16O	64
6.	Fenchone	152	C10H16O	45
7.	Cyclohexanol, 4-(1-methylethyl)-	142	C9H18O	39
8.	TRANS,TRANS-NONA-2,4-DIENAL	138	C9H14O	33
9.	(-)-Epicamphor	152	C10H16O	12
10.	1H-Inden-1-one, octahydro-7a-methyl-, ci	152	C10H16O	9
11.	Pulegone	152	C10H16O	9
12.	Fenchone	152	C10H16O	6
13.	Fenchone	152	C10H16O	6

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*83	001195-79-5	124016	60	27	1	99	14	50	0	56	9907
2.	*74	004695-62-9	124010	69	17	0	90	16	44	11	58	9865
3.	*72	004695-62-9	13780	55	31	1	93	20	42	0	49	9860
4.	*64	001195-79-5	124011	55	29	0	96	19	37	5	40	9890
5.	*64	001195-79-5	13781	45	42	3	91	24	37	0	44	9855
6.	*45	001195-79-5	124015	40	51	1	89	22	19	0	33	9873
7.	39	004621-04-9	10226	36	61	2	76	19	15	0	21	9205
8.	33	005910-87-2	122256	34	45	2	92	33	10	1	23	8694
9.	*12	010292-98-5	13789	39	61	1	52	62	2	0	35	9267
10.	* 9	013025-91-7	13741	30	47	0	24	80	1	0	33	8288
11.	* 9	000089-82-7	123990	30	48	0	13	74	1	0	33	7259
12.	* 6	001195-79-5	124014	27	83	2	65	74	1	1	18	9240
13.	* 6	001195-79-5	124013	27	83	2	65	74	1	1	18	9239

Peak 141



Scan 1482 (29.061 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	6277	61.05	39	71.00	4543	84.05	260
50.95	92	61.95	41	72.00	223	86.95	6
51.95	123	62.25	66	73.00	76	88.30	26
52.95	1719	62.90	7	74.10	21	91.00	2977
53.95	170	63.90	68	77.05	1664	92.00	1049
54.95	6156	65.00	792	78.05	354	93.00	4633
55.95	843	66.00	268	78.95	3807	94.00	2384
57.05	1602	67.00	3928	79.95	2769	95.00	6529
57.95	267	68.00	796	81.05	7627	96.00	714
58.95	31	69.00	5997	82.05	1323	97.10	1504
60.05	125	70.00	724	83.05	1208	98.05	231

Scan 1482 (29.061 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
100.10	21	112.05	55	123.15	2699	135.05	1360
102.10	63	113.05	17	124.15	482	136.05	1281
102.95	128	114.05	51	125.15	15	137.05	5350
103.95	102	115.05	297	126.05	74	138.05	815
105.05	2206	116.00	71	128.00	11	139.05	90
106.05	1047	117.00	348	129.00	101	141.05	94
107.05	3673	118.00	118	130.00	66	142.10	14
108.05	1105	119.00	1773	131.05	426	143.00	71
109.05	2719	120.15	889	132.05	237	145.15	350
110.05	272	121.00	2568	133.05	1410	146.00	73
111.05	467	122.00	763	134.05	1872	147.15	850

Scan 1482 (29.061 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
148.15	796	162.05	195	174.10	98	188.05	171
149.10	622	163.05	668	175.15	765	189.05	766
150.15	239	164.10	118	176.15	497	190.20	1070
151.05	69	165.05	181	177.15	1307	191.20	550
152.15	4	166.15	46	178.15	181	192.20	173
153.15	92	168.20	42	182.10	16	194.10	6
154.15	107	169.00	63	183.05	52	195.10	103
156.20	10	170.00	25	184.05	37	197.00	23
159.05	335	171.00	33	185.05	36	199.10	18
160.15	120	172.00	55	186.05	8	200.10	15
161.05	884	173.15	153	187.05	529	201.15	368

Scan 1482 (29.061 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
202.25	624	215.15	179	228.05	29	246.20	29
203.15	860	216.25	178	229.15	320	247.20	18
204.15	509	219.10	69	230.20	145	248.05	4
205.15	88	220.05	19	231.30	66	249.45	56
207.15	21	221.30	155	236.00	31	251.10	23
208.25	34	222.45	17	237.20	95	252.30	5
208.90	86	224.90	21	238.20	47	253.15	16
209.75	45	226.15	32	241.10	37	255.25	112
210.25	45	227.00	28	243.30	189	256.20	9
211.20	39	227.25	37	244.20	692	257.25	1838
211.95	19	227.65	22	245.20	189	258.35	288

Scan 1482 (29.061 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
261.90	19						
262.45	17						
262.75	20						
264.25	13						
265.20	21						
267.25	21						
270.20	54						
271.20	54						
272.20	655						
273.45	131						
274.25	34						

Scan 1482 (29.061 min): A1873.D

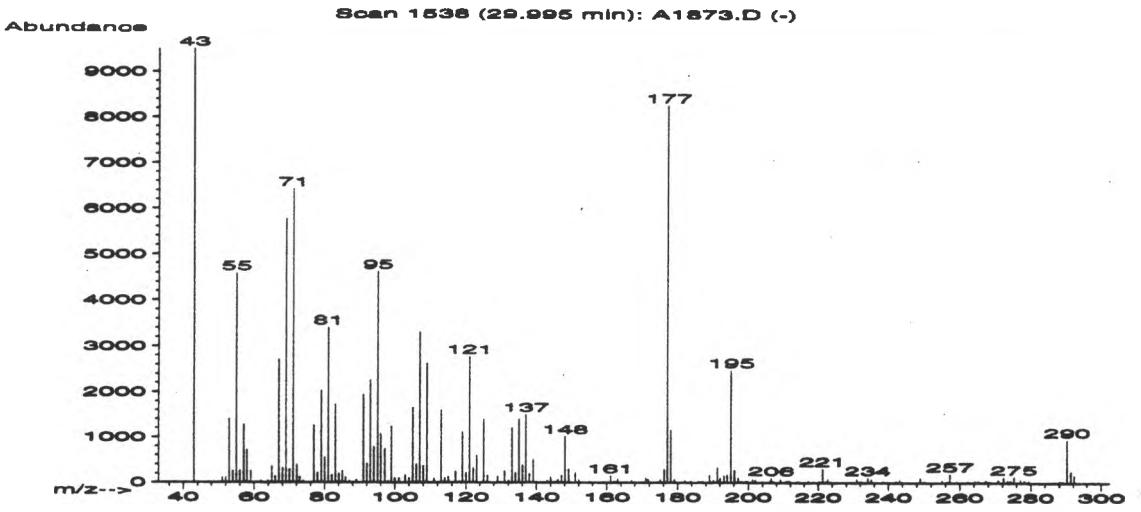
PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	1-Naphthalenepropanol, .alpha.-ethenylde	306	C20H34O2	58
2.	1-Naphthalenepropanol, .alpha.-ethenylde	306	C20H34O2	43
3.	Naphthalene, 2-butyldecahydro-	194	C14H26	35
4.	DECAHYDRO-2-ETHYL-NAPHTHALENE	166	C12H22	27
5.	4,4-Dimethyl-5-ethylcyclopent-2-en-1-one	138	C9H14O	27
6.	Cyclohexene, 1-methyl-4-(1,5,9-trimethyl	272	C20H32	25
7.	(3.alpha.,6a.alpha.,6b.alpha.,9.beta.,12	272	C18H24O2	18
8.	2(1H)-Pyridinone, 1-propyl-	137	C8H11NO	14
9.	1H-Pyrrole, 1-pentyl-	137	C9H15N	14
10.	19-DI-TORULOSOL	306	C20H33DO2	14
11.	(-)-Nerolidol	222	C15H26O	11
12.	SANDARACOPIMAR-15-ENE-8.BETA.-YL-ACETATE	332	C22H36O2	11
13.	13-Epimanool	290	C20H34O	11
14.	Sclareol	308	C20H36O2	10
15.	Cyclohexene, 3-methyl-6-(1-methylethyl)-	138	C10H18	10
16.	N-ISOPENTYLIDENE FURFURYL AMINE	165	C10H15NO	10
17.	Dendrolasin	218	C15H22O	10
18.	CYCLOPROPANCARBONIC ACID, 2,2-DIMETHYL-3	140	C8H12O2	10
19.	Nerolidol	222	C15H26O	10
20.	(R)-(-)-Cembrene	272	C20H32	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	58	003650-30-4	75935	125	44	1	85	33	32	35	52	7726
2.	43	004549-12-6	75934	108	48	1	80	45	18	11	39	7615
3.	35	006305-52-8	127888	78	31	0	99	51	11	12	41	7922
4.	27	000000-00-0	19756	54	55	1	95	60	8	6	39	7952
5.	27	081825-20-9	8610	53	50	0	85	56	8	23	40	6921
6.	*25	056248-11-4	64431	48	130	3	76	65	7	0	44	7244
7.	*18	071370-28-0	64349	69	118	3	66	70	3	0	44	5983
8.	*14	019006-63-4	8281	55	66	3	66	69	2	14	39	6529
9.	*14	000699-22-9	8321	47	59	1	98	68	2	0	39	7067
10.	14	001438-63-7	75943	102	78	1	82	68	2	0	41	7789
11.	*11	017430-12-5	44949	46	49	0	72	74	2	0	44	6186
12.	11	041756-14-3	83626	78	98	2	82	75	2	0	43	6589
13.	11	001438-62-6	70744	75	97	0	50	75	2	0	45	6605
14.	10	000515-03-7	133720	77	100	2	36	75	1	0	41	8640
15.	*10	005256-65-5	8795	34	68	0	60	79	1	0	41	4834
16.	*10	000000-00-0	18995	38	35	0	98	75	1	0	39	5722

17.	10	023262-34-2	42953	44	81	0	62	76	1	0	39	7050
18.	10	067528-58-9	9193	47	64	0	81	80	1	0	39	4655
19.	*10	007212-44-4	129867	39	57	0	72	74	1	0	39	6186
20.	*10	079355-93-4	64435	59	57	0	43	79	1	19	43	4387

Peak 142



Scan 1538 (29.995 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	9501	63.90	44	76.95	1262	88.95	65
50.95	105	65.00	363	77.95	219	91.00	1945
51.95	104	66.00	136	79.05	2035	92.00	416
52.95	1398	67.00	2706	80.05	555	93.00	2274
53.95	251	68.00	325	81.05	3405	94.00	794
54.95	4586	69.00	5776	82.05	160	95.05	4619
55.95	270	70.00	296	83.05	1725	96.00	1077
57.05	1282	71.00	6426	84.05	198	97.15	743
58.00	723	72.10	400	85.05	254	98.05	30
59.05	264	72.95	122	85.95	110	99.00	1236
61.90	38	73.95	44	87.05	32	100.00	88

Scan 1538 (29.995 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
101.05	94	115.05	120	129.95	11	143.00	44
102.95	172	117.00	249	131.00	261	144.00	110
104.00	101	118.00	12	132.05	47	145.15	19
105.00	1667	119.00	1112	133.05	1212	146.00	62
106.00	412	120.00	218	134.05	217	147.10	165
107.05	3309	121.00	2775	135.05	1404	148.15	1018
108.05	375	122.10	324	136.05	388	149.15	302
109.05	2631	123.10	595	137.05	1508	151.00	219
111.05	84	125.10	1403	138.05	187	152.05	65
113.05	1597	126.15	153	139.10	505	155.05	35
114.05	93	129.10	136	140.00	21	157.00	8

Scan 1538 (29.995 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
159.05	13	178.15	1158	193.15	150	204.15	28
161.05	153	179.15	70	194.05	166	206.20	33
162.05	24	182.05	50	195.20	2486	206.50	107
163.10	83	183.25	10	196.20	283	207.15	33
167.10	41	183.80	36	197.15	95	209.15	78
171.00	99	186.05	27	198.15	29	210.25	14
171.50	60	187.05	37	199.05	19	210.95	40
171.75	72	189.05	159	199.65	33	211.55	34
175.10	63	190.10	48	201.20	71	211.80	35
176.20	286	191.20	342	202.00	57	214.05	30
177.15	8263	192.10	96	203.15	8	217.20	34

Scan 1538 (29.995 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
220.25	27	249.05	103	267.95	19	288.90	30

221.20	309	250.25	17	268.20	4	290.25	963
222.25	20	255.00	47	270.80	55	291.30	253
222.80	75	256.40	29	272.25	121	292.30	160
231.00	78	257.25	196	273.45	50		
232.15	28	259.05	17	274.30	45		
234.15	113	262.20	17	275.25	135		
235.20	68	264.20	32	277.05	61		
238.45	17	265.05	37	278.20	47		
242.05	36	266.55	13	279.40	36		
243.20	59	267.30	57	288.15	39		

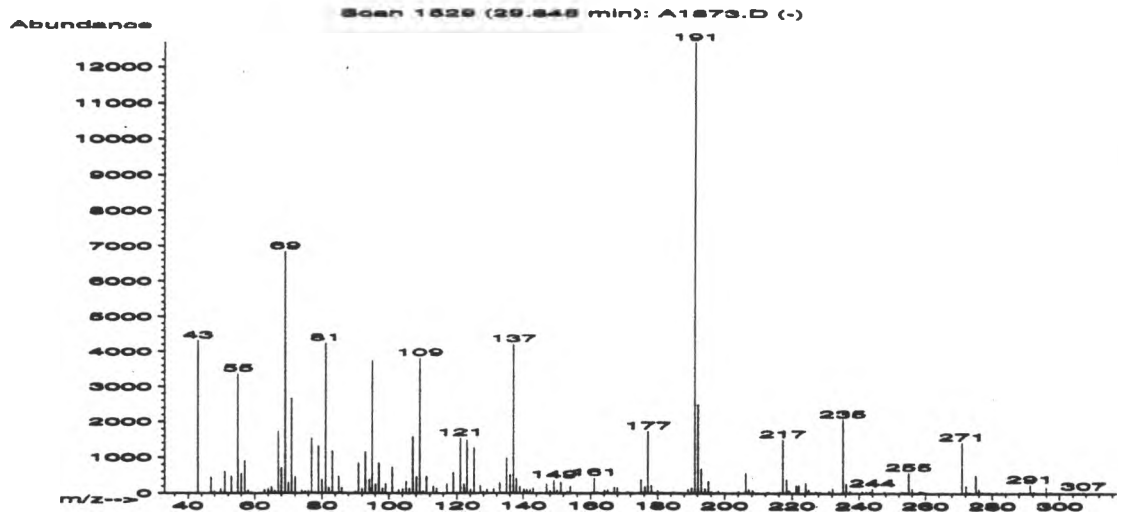
Scan 1538 (29.995 min): A1873.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	(11E,13Z)-11813-LABDADIEN-8-OL	290	C20H34O	59
2.	S-Triazolo(1,5-A)pyrimidine, 5-methyl-7-	177	C8H11N5	35
3.	2,2-Dimethyl-4-azahomoadamant-4-enes	177	C12H19N	27
4.	.beta.-Ionone	192	C13H20O	25
5.	2-Pyrimidinamine, 4-methyl-6-(trifluorom	177	C6H6F3N3	22
6.	1H-Indazole, 1-methyl-4-nitro-	177	C8H7N3O2	22
7.	Phenol, 2,4-bis(1-methylpropyl)-	206	C14H22O	22
8.	1,3-Benzodioxol-2-one, 5-(1,1-dimethylet	192	C11H12O3	22
9.	3H-1,2,4-Triazole-3-thione, 1,2-dihydro-	177	C8H7N3S	22
10.	EDULAN II	192	C13H20O	16
11.	4-Azatetracyclo[6.3.1.0(2,6)0(5,10]dodec	177	C11H15NO	16
12.	2,5,5,8A-TETRAMETHYL-6,7,8,8A-TETRAHYDRO	192	C13H20O	12
13.	Phenol, bis(1-methylpropyl)-	206	C14H22O	12
14.	4-Pyrimidinamine, 2-methyl-6-(trifluorom	177	C6H6F3N3	12
15.	EDULAN IV	192	C13H20O	12
16.	6.BETA.-HYDROXY-4,8.ALPHA.,11.BETA.-TRIM	290	C20H34O	11
17.	(-)-2.BETA.-HYDROXYVERRUCOSANE	290	C20H34O	10
18.	2(5H)-Furanone, 3,5-dimethyl-5-[(4-methy	220	C12H12O4	10
19.	Phenol, 2,5-bis(1-methylpropyl)-	206	C14H22O	10
20.	(3.alpha.,5.beta.,6.alpha.)-3,6-Dihydrox	334	C21H34O3	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*59	000000-00-0	70760	67	105	3	60	23	33	0	39	9807
2.	*35	051806-90-7	24149	33	82	3	86	54	11	0	39	7138
3.	*27	088537-06-8	126535	43	77	2	62	57	8	0	40	7070
4.	25	014901-07-6	127734	59	69	2	63	53	7	8	35	7225
5.	*22	005734-63-4	24098	34	79	1	79	64	5	0	39	6615
6.	*22	026120-43-4	24126	36	80	2	64	65	5	0	39	6580
7.	22	001849-18-9	37566	45	57	2	60	62	5	9	38	6705
8.	22	054815-21-3	30741	47	55	3	81	65	5	0	39	6583
9.	*22	003414-94-6	24142	33	80	2	63	65	5	0	39	6582
10.	16	041678-30-2	31040	59	65	2	66	57	3	0	36	6958
11.	*16	081569-81-5	24289	37	37	2	70	59	3	15	36	6584
12.	12	005552-30-7	31037	53	35	1	77	65	2	0	37	6585
13.	12	031291-60-8	128860	50	51	2	57	63	2	0	35	6714
14.	*12	054518-10-4	24097	38	66	1	60	63	2	0	35	6661
15.	12	000000-00-0	31042	47	89	2	87	61	2	0	35	6983
16.	*11	068420-55-3	70762	43	121	3	82	80	2	0	44	3709
17.	*10	069770-76-9	70763	35	81	3	116	73	1	0	39	4528
18.	10	041763-40-0	43581	46	81	2	50	76	1	0	39	6656
19.	*10	054932-77-3	37567	35	59	2	42	75	1	11	40	6714
20.	10	000000-00-0	84189	43	25	0	93	76	1	0	39	5528

Peak 143



Scan 1529 (29.845 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	4309	58.95	42	74.05	92	85.95	155
46.90	449	62.90	113	75.00	70	86.95	15
47.90	61	64.00	129	76.00	69	88.00	15
49.80	129	65.00	194	76.95	1543	90.15	62
50.95	601	66.00	78	77.95	37	91.00	845
51.95	24	67.00	1730	79.00	1313	92.00	132
52.95	486	68.00	714	80.05	373	93.00	1148
54.95	3366	69.00	6847	81.05	4250	94.15	388
55.95	558	70.00	315	82.05	158	95.00	3751
57.05	916	71.00	2664	83.05	1173	96.05	259
57.95	95	72.00	465	85.05	476	97.00	853

Scan 1529 (29.845 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
98.05	147	111.05	480	125.15	1288	139.05	198
99.05	280	113.05	207	127.05	224	140.20	123
101.00	742	114.05	145	128.00	59	141.05	112
102.95	103	115.95	10	129.05	126	142.05	104
104.05	133	117.00	263	131.05	133	143.00	157
105.00	340	119.00	584	133.05	303	147.00	271
106.05	152	120.00	26	134.05	30	148.05	83
107.05	1597	121.10	1550	135.05	996	149.15	368
108.05	458	122.10	260	136.05	524	150.10	93
109.05	3818	123.05	1486	137.05	4218	151.15	321
110.05	76	124.10	112	138.05	417	153.15	54

Scan 1529 (29.845 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
154.00	204	172.10	15	185.05	53	200.05	30
155.20	11	175.05	385	189.15	124	204.05	68
160.00	18	176.15	190	190.20	171	206.25	567
161.10	430	177.15	1730	191.20	12683	207.15	112
162.00	37	178.20	230	192.20	2491	208.25	98
164.05	93	179.10	24	193.15	693	212.70	52
165.05	104	180.00	94	194.20	143	216.20	44
167.10	182	181.20	32	195.20	340	217.20	1496
168.05	175	182.00	15	196.15	48	218.30	384
169.20	6	183.15	13	197.15	6	219.05	87
171.10	46	184.20	33	198.15	76	221.20	229

Scan 1529 (29.845 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
222.05	231	242.05	58	258.00	58	275.05	515

224.15	293	243.20	64	258.40	60	276.05	122
225.15	102	244.05	138	259.15	62	277.05	47
227.15	58	247.70	53	260.00	31	279.25	37
228.50	37	250.20	38	262.10	4	281.40	24
231.15	77	252.40	25	264.25	2	288.20	48
232.15	139	253.15	58	264.95	34	289.15	39
235.25	2068	254.15	35	266.70	23	290.25	36
236.25	273	255.00	573	270.95	1425	291.20	250
237.25	72	256.00	133	272.20	208	292.20	54
240.95	70	257.15	16	273.20	31	293.05	42

Scan 1529 (29.845 min): A1873.D

Modified:subtracted clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
295.95	174						
297.30	46						
303.05	26						
304.20	30						
306.15	26						
307.15	58						

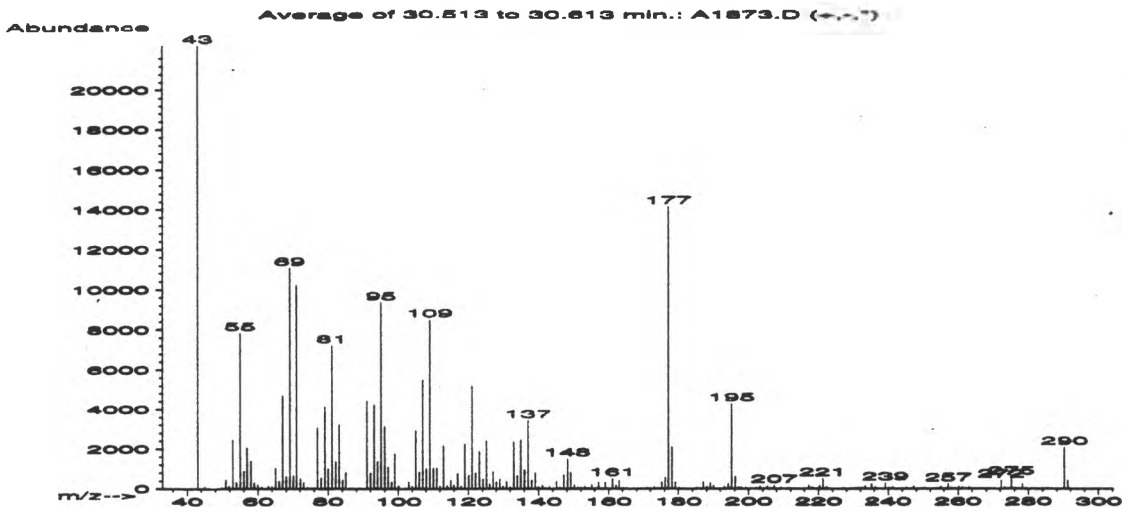
Scan 1529 (29.845 min): A1873.D

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	8,12.XI.-EPOXYLABD-14-EN-13.XI.-OL UNIDE	306	C20H34O2	78
2.	8,12.XI.-EPOXYLABD-14-EN-13.XI.-OL UNIDE	306	C20H34O2	64
3.	1,1,3,3-TETRAMETHYL-1,3-DISILAINDAN	206	C11H18Si2	59
4.	8,12.XI.-EPOXYLABD-14-EN-13.XI.-OL UNIDE	306	C20H34O2	50
5.	1,3,4,7,7-PENTAMETHYL-2-OXA-BICYCLO(4,4,	206	C14H22O	43
6.	1-(PHENYLTHIOXOMETHYL)PYRROLIDINE	191	C11H13NS	43
7.	Phenanthrene, 9-dodecyltetradecahydro-	360	C26H48	38
8.	(Z)-4-(2',6',6'-Trimethyl-1'-cyclohexen-	206	C14H22O	35
9.	Oxirane, [[4-(1,1-dimethylethyl)phenoxy]	206	C13H18O2	32
10.	2-(PHENYLAMINO)-5,6-DIHYDRO-(4H)-1,3-THI	192	C10H12N2S	18
11.	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	11
12.	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	10
13.	2,6,10,15,19,23-HEXAMETHYL-2,6,10,14,18,	410	C30H50	10
14.	Tricyclo[4.3.0.0(7,9)]nonane, 2,2,5,5,8,	206	C15H26	10
15.	Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	9
16.	10,10-Dimethyl-2-trans- 7-cis-tricyclo-[	192	C13H20O	9
17.	1,1':3',1''-Tercyclopentane	206	C15H26	9
18.	Anthracene, 9-cyclohexyltetradecahydro-	274	C20H34	9
19.	2,6,10,14,18,22-Tetracosahexaene, 2,6,10	410	C30H50	9
20.	4-Methylspiro(4.7)dodec-3-en-1-one	192	C13H20O	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	78	056711-40-1	75961	53	38	0	72	10	46	5	41	9916
2.	64	056711-39-8	75960	65	26	0	76	10	37	1	37	9918
3.*	59	054113-93-8	37331	30	45	1	81	25	33	20	38	8660
4.	50	056682-25-8	75958	57	40	0	53	35	25	0	39	9815
5.*	43	000000-00-0	37704	49	65	3	99	47	18	0	46	8661
6.*	43	015563-45-8	30380	37	60	2	99	50	18	14	43	8649
7.	38	055334-01-5	135234	57	93	2	72	40	14	3	37	8713
8.*	35	089128-16-5	37620	33	48	2	67	52	11	0	39	8665
9.	32	003101-60-8	128852	43	77	3	97	50	9	0	35	8497
10.*	18	003420-40-4	30693	34	44	0	47	70	3	23	43	8511
11.*	11	000096-76-4	128861	35	62	1	61	75	2	9	43	8612
12.*	10	000096-76-4	128862	43	50	1	56	75	1	20	40	8619
13.	10	000000-00-0	99541	56	81	3	187	78	1	0	39	4941
14.	10	054832-82-5	37766	42	85	2	64	62	1	6	29	7709
15.*	9	000096-76-4	128866	36	60	1	50	75	1	14	35	8625
16.*	9	077983-56-3	31076	44	66	2	34	80	1	0	35	3010
17.*	9	006051-40-7	37760	34	78	2	35	76	1	0	35	3990
18.	9	055255-70-4	132392	44	89	2	32	75	1	0	37	8525
19.	9	007683-64-9	99537	46	93	2	178	80	1	0	37	5028
20.*	9	088441-59-2	31021	37	71	2	35	80	1	0	30	3045

Peak 144



Average of 30.513 to 30.613 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	22263	58.00	1407	67.00	4686	76.95	3084
45.00	117	58.95	319	68.00	625	77.95	547
47.65	4	59.95	212	69.00	11093	79.05	4144
49.85	74	61.00	108	70.00	672	80.00	1012
50.95	492	61.65	4	71.00	10257	81.05	7230
51.90	153	62.00	16	72.05	530	82.05	1376
52.95	2469	62.95	150	73.00	310	83.05	3231
53.95	336	63.70	16	74.05	73	84.05	448
54.95	7847	63.95	104	75.00	52	85.05	823
56.00	890	65.00	1042	75.70	19	86.00	40
56.95	2067	66.00	378	76.00	74	87.05	48

Average of 30.513 to 30.613 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
88.05	40	100.05	167	112.05	145	123.10	1900
88.95	65	102.05	18	113.05	2164	124.15	497
91.00	4433	103.00	336	114.05	168	125.15	2424
92.00	786	104.00	149	115.05	441	126.10	251
93.00	4264	105.05	2933	116.00	194	127.10	864
94.00	1394	106.05	840	117.00	758	128.05	346
95.00	9370	107.05	5521	118.00	152	129.10	487
96.05	3143	108.05	1026	119.00	2245	130.00	151
97.05	1100	109.05	8519	120.05	681	131.05	368
98.05	337	110.05	1058	121.00	5215	132.05	109
99.00	1767	111.05	1049	122.05	794	133.05	2366

Average of 30.513 to 30.613 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
134.05	657	145.05	380	156.10	58	167.10	44
135.05	2460	146.05	94	157.05	347	168.25	45
136.05	965	147.10	719	158.05	60	168.55	10
137.05	3457	148.15	1530	159.05	322	169.15	42
138.10	438	149.15	837	160.10	44	169.95	21
139.10	813	150.10	198	161.10	523	171.05	82
140.05	109	151.10	85	162.10	170	172.05	21
141.10	178	152.15	91	163.10	420	173.05	106
142.05	73	153.15	133	164.15	73	174.10	28
143.00	122	154.10	55	165.05	42	175.15	362
144.10	26	155.20	210	166.05	19	176.15	574

Average of 30.513 to 30.613 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
177.15	14156	188.10	116	200.30	28	211.25	36
178.15	2104	189.10	290	202.15	47	215.95	10
179.15	357	190.10	159	203.20	135	216.20	4
180.10	68	193.15	102	204.20	27	217.20	199
181.15	17	194.25	241	205.20	133	218.15	92
182.20	18	195.20	4287	206.20	25	219.20	44
183.10	2	196.20	627	207.25	170	220.25	163
183.70	10	197.20	88	208.20	13	221.25	531
185.10	67	198.00	79	209.20	76	222.25	105
186.05	37	199.15	62	210.25	6	223.55	8
187.10	352	200.10	7	210.55	1	223.85	6

Average of 30.513 to 30.613 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
224.20	13	237.80	13	250.40	18	262.20	26
225.10	13	239.20	301	251.15	11	263.20	88
227.20	14	240.20	47	255.10	120	264.05	12
229.20	31	241.25	95	255.55	24	264.30	14
230.30	45	242.50	3	256.35	21	265.60	8
231.20	67	243.15	3	257.20	243	267.45	5
232.20	47	244.00	7	258.15	41	267.90	4
233.30	154	245.20	62	259.15	42	268.35	9
234.25	13	247.30	127	260.20	119	270.20	26
235.20	251	248.30	36	260.75	6	270.80	3
236.25	69	249.25	30	261.25	100	271.30	5

Average of 30.513 to 30.613 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
272.25	448	281.20	18	291.30	438		
273.25	93	281.45	11	292.20	24		
274.05	5	282.00	5	292.70	7		
274.25	21	282.75	2	293.95	3		
275.10	594	284.20	24	294.35	14		
276.20	50	284.50	18				
277.20	23	285.50	2				
278.25	245	286.40	10				
279.15	11	287.90	4				
279.35	44	288.25	2				
280.50	2	290.25	2094				

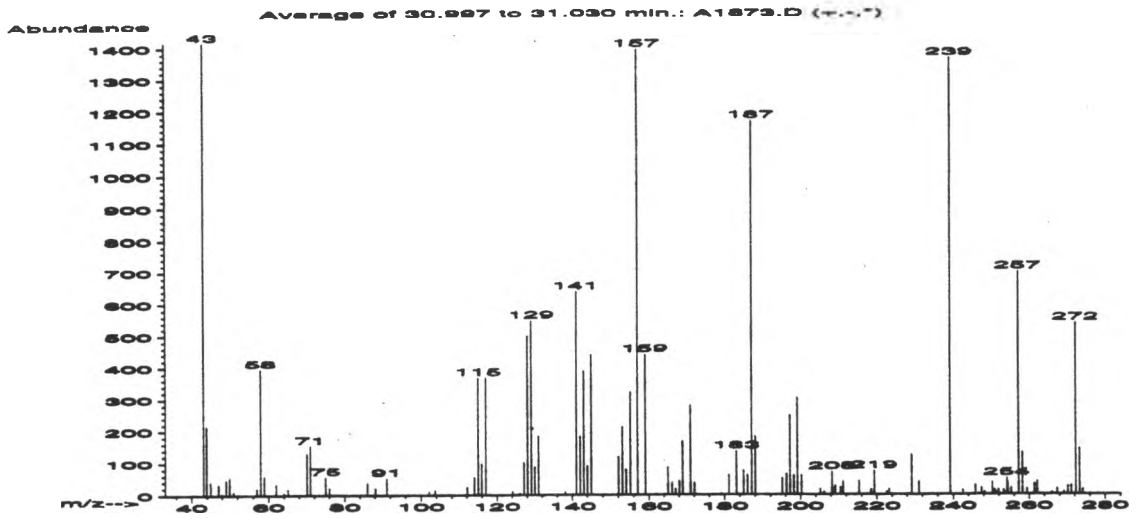
Average of 30.513 to 30.613 min.: A1873.D
Converted from RTE data file: >A1873:

PBM Search of library D:\DATABASE\WILEY138.L

	Name	MolWt	Formula	Qual
1.	(11E,13Z)-11813-LABDADIEN-8-OL	290	C20H34O	55
2.	(+-)gymnomitrol	220	C15H24O	16
3.	3,4,5,6-TETRAMETHYL-2,5-OCTADIENE	166	C12H22	14
4.	2,2-Dimethyl-4-azahomoadamant-4-enes	177	C12H19N	14
5.	7-amino-3-methylpyrimido(4,5-c)pyridazin	177	C7H7N5O	12
6.	trans-.beta.-Ionone	192	C13H20O	10
7.	Androstan-11-one, 3-hydroxy-, (3.beta.,5	290	C19H30O2	10
8.	4-Azatetracyclo[6.3.1.0(2,6)0(5,10]dodec	177	C11H15NO	10
9.	Lanostan-3-one, 11.beta.,18-epoxy-	442	C30H50O2	10
10.	2,5,5,8A-TETRAMETHYL-6,7,8,8A-TETRAHYDRO	192	C13H20O	10
11.	4(ax)-Aminoadamantane-2(ax)-carboxylic a	195	C11H17NO2	10
12.	1H-Indazole, 1-methyl-4-nitro-	177	C8H7N3O2	10
13.	Isogeraniol	154	C10H18O	10
14.	.beta.-Ionone	192	C13H20O	10
15.	3-METHYLAMINO-1-PHENYL-2-PROPENE-1-THION	177	C10H11NS	10
16.	Silane, tributylchloro-	234	C12H27ClSi	10
17.	(3.alpha.,5.beta.,6.alpha.)-3,6-Dihydrox	334	C21H34O3	10
18.	4-Pyrimidinamine, 2-methyl-6-(trifluorom	177	C6H6F3N3	10
19.	2-METHOXY-13C-3-METHYLPYRAZINE	124	C513CH8N2O	10
20.	2-Pyrimidinamine, 4-methyl-6-(trifluorom	177	C6H6F3N3	10

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*55	000000-00-0	70760	79	67	1	34	45	29	0	78	9785
2.	16	071564-38-0	43988	41	35	0	53	58	3	13	35	5920
3.	14	000000-00-0	19728	44	34	0	37	70	2	14	41	4556
4.	*14	088537-06-8	126535	46	73	2	54	70	2	0	39	6581
5.	*12	074482-47-6	24108	33	54	1	61	62	2	0	35	6617
6.	10	000079-77-6	31004	47	63	1	50	69	1	0	37	6836
7.	*10	000570-27-4	70685	40	102	0	20	75	1	22	40	7971
8.	*10	081569-81-5	24289	37	42	2	57	75	1	0	39	6148
9.	10	025116-73-8	103818	43	148	0	39	75	1	0	39	5867
10.	10	005552-30-7	31037	44	43	1	77	75	1	0	39	6238
11.	*10	081601-64-1	32371	37	48	0	29	77	1	0	41	6266
12.	*10	026120-43-4	24126	36	80	1	55	79	1	0	39	6142
13.	10	005944-20-7	14595	69	35	1	32	77	1	0	38	5362
14.	10	014901-07-6	127735	46	61	1	53	69	1	0	37	6848
15.	*10	054920-39-7	24229	33	81	2	59	78	1	0	39	6184
16.	10	000995-45-9	49836	57	61	0	29	80	1	0	39	6904
17.	10	000000-00-0	84189	43	25	0	72	79	1	0	39	5571
18.	*10	054518-10-4	24097	47	56	1	59	75	1	0	40	6311
19.	10	034061-82-0	4673	53	100	2	31	70	1	16	37	5647
20.	*10	005734-63-4	24098	34	78	1	63	78	1	0	39	6189

Peak 145



Average of 30.997 to 31.030 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
43.00	1417	61.70	3	102.05	12	128.05	500
43.90	215	61.95	33	103.70	15	129.10	549
44.90	40	63.90	7	112.10	25	130.00	89
47.00	33	65.00	19	113.95	54	131.05	185
48.00	5	70.05	129	115.00	367	138.10	10
49.00	47	71.00	154	115.95	98	140.05	2
49.90	53	75.00	55	117.00	368	141.05	639
50.95	11	76.00	21	124.10	12	142.05	184
57.00	20	86.05	38	125.15	2	143.00	388
57.95	395	88.10	21	126.05	5	144.00	91
58.95	57	91.00	52	127.15	102	145.00	440

Average of 30.997 to 31.030 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
152.10	119	171.05	280	197.20	249	218.45	16
153.15	212	172.05	38	198.25	61	219.30	74
154.10	80	179.10	5	199.15	304	222.55	9
155.15	323	181.15	62	200.25	61	223.25	18
157.05	1395	183.10	136	205.20	17	224.10	2
159.05	441	185.00	76	206.20	8	227.95	3
165.05	87	186.00	62	208.30	71	229.20	124
166.10	38	187.15	1168	209.15	27	231.15	40
167.05	19	188.05	182	210.50	22	239.20	1366
168.10	44	195.15	51	211.15	40	242.55	14
169.05	168	196.30	65	215.30	42	245.80	29

Average of 30.997 to 31.030 min.: A1873.D
Converted from RTE data file: >A1873:
Modified:added subtracted scaled clipped

m/z	abund.	m/z	abund.	m/z	abund.	m/z	abund.
247.45	20	258.20	131	274.10	16		
248.25	7	259.40	18				
250.30	39	261.40	33				
250.80	15	262.10	41				
251.05	10	265.85	6				
251.90	15	267.30	19				
253.25	14	269.05	9				
254.10	50	270.10	26				
254.40	38	271.05	28				
255.20	19	272.25	539				
257.20	701	273.25	144				

Average of 30.997 to 31.030 min.: A1873.D
Converted from RTE data file: >A1873:

PBM Search of library D:\DATABASE\WILEY138.L

BKME Supplimental [4]

	Name	MolWt	Formula	Qual
1.	4-Androsten-3-one	272	C19H28O	22
2.	2-Propenoic acid, 3-(1H-indol-3-yl)-	187	C11H9NO2	15
3.	Androst-8-en-11-one, (5.alpha.)-	272	C19H28O	11
4.	Quinoline, 2,6-dimethyl-	157	C11H11N	11
5.	3,6-DIMETHYLQUINOLINE	157	C11H11N	11
6.	N-(P-TOLYL)MALEIMIDE	187	C11H9NO2	10
7.	2-Propenoic acid, 2-cyano-3-phenyl-, met	187	C11H9NO2	10
8.	Quinoline, 2,3-dimethyl-	157	C11H11N	10
9.	Quinoline, 2,4-dimethyl-	157	C11H11N	10
10.	1,3,4-Trimethyl-2,3-dihydro-1H-1-benzaze	187	C13H17N	10
11.	Quinoline, 2,6-dimethyl-	157	C11H11N	10
12.	Quinoline, 2,6-dimethyl-	157	C11H11N	10
13.	2-N-BUTYL-8-N-HEXYL-1,2,3,4-TETRAHYDRONA	272	C20H32	10
14.	Quinoline, 2,7-dimethyl-	157	C11H11N	10
15.	2-[(BUTYLDIMETHYLSILYL)OXY]-2-PENTEN-4-O	214	C11H22O2Si	9
16.	3-Penten-2-one, 4-chloro-1,1,1,5,5,5-hex	226	C5HClF6O	9
17.	2-Furoic acid, 5-bromo-3-methyl-, methyl	218	C7H7BrO3	9
18.	Acetic acid, (3-methyl-4-oxo-2-thiazolid	187	C7H9NO3S	9
19.	1H-Indole, 2-(tetrahydro-2-furanyl)-	187	C12H13NO	9
20.	4-CHLORO-6-HYDROXY-2,3-LUTIDINE	157	C7H8ClNO	9

	Prob	CAS#	Ref#	K	dK	Flag	%	Con	C_1	Tilt	R_IV	XCORR
1.	*22	002872-90-4	132272	37	132	1	74	64	5	0	39	7368
2.	*15	001204-06-4	28816	58	63	1	66	78	2	0	56	4782
3.	*11	054498-82-7	64401	33	69	0	38	80	2	2	43	3456
4.	*11	000877-43-0	124636	46	56	0	98	78	2	0	44	5529
5.	*11	000000-00-0	15846	47	59	0	75	78	2	0	44	5582
6.	*10	001631-28-3	127433	33	103	2	77	80	1	0	39	4479
7.	*10	003695-84-9	28806	34	83	2	62	79	1	5	40	5182
8.	*10	001721-89-7	15842	47	54	2	98	79	1	0	40	5448
9.	*10	001198-37-4	124632	33	62	0	98	79	1	0	41	5518
10.	*10	057091-68-6	28894	37	54	0	63	80	1	0	41	4479
11.	*10	000877-43-0	124637	40	61	0	98	78	1	0	39	5545
12.	*10	000877-43-0	124634	34	65	0	98	78	1	0	41	5512
13.	*10	000000-00-0	64452	36	95	3	336	80	1	0	41	4998
14.	*10	000093-37-8	15845	34	67	0	90	79	1	0	41	5515
15.	9	000000-00-0	41147	46	82	2	84	76	1	0	37	5472
16.	9	056666-71-8	46339	45	70	1	91	71	1	0	37	5749
17.	9	002528-01-0	42497	43	98	2	72	80	1	0	35	4479
18.	* 9	056196-67-9	28703	28	65	0	82	80	1	6	35	5042
19.	* 9	050640-01-2	28868	42	66	2	69	79	1	1	36	4717
20.	* 9	000000-00-0	15710	34	73	2	98	78	1	0	35	5563