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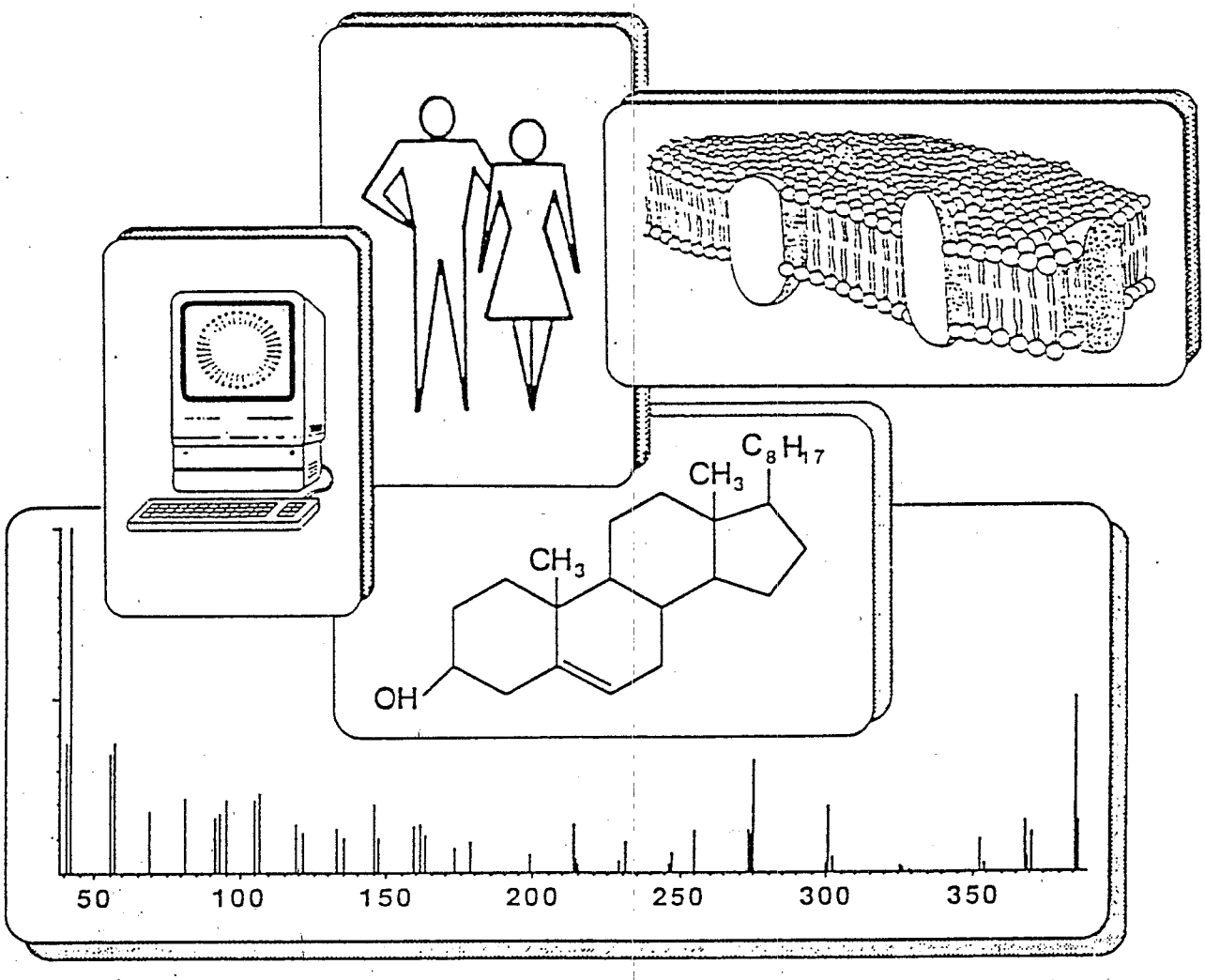
CHARACTERIZATION OF HRGC/MS UNIDENTIFIED PEAKS FROM THE ANALYSIS OF HUMAN ADIPOSE TISSUE

VOLUME I - TECHNICAL APPROACH



CHARACTERIZATION OF HRGC/MS UNIDENTIFIED PEAKS FROM THE ANALYSIS OF HUMAN ADIPOSE TISSUE

VOLUME I: TECHNICAL APPROACH

by

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FINAL REPORT

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PREFACE

This report describes Midwest Research Institute's approach to characterize unidentified chromatographic peaks in HRGC/MS data collected from the analysis of human adipose tissue for general volatile and semivolatile organic compounds. This report is provided as two separate volumes. Volume I describes the technical approach and presents a summary of the results based on frequency of observation by age group and census region. Volume II is an appendix to Volume I and contains additional details on frequency of occurrence for both identified and unidentified peaks based on census region, census division, and age. This report focuses on the approach to identifying compounds from the HRGC/MS spectra. The frequency of detection of specific compounds is presented. The HRGC/MS data were collected for 46 samples prepared as composites from individual specimens of the U.S. Environmental Protection Agency's fiscal year 1982 (FY82) National Human Adipose Tissue Survey (NHATS) repository. The sample collection, compositing, and the analysis of the composites for specific volatile and semivolatile organic compounds are described in detail in separate reports (Stanley 1986b, Stanley 1986c).

This approach to the characterization of HRGC/MS unidentified peaks was developed and conducted for the EPA's Office of Toxic Substances, Field Studies Branch (EPA Contract No. 68-02-4252, Work Assignment 23, Ms. Janet Remmers, Work Assignment Manager, and Dr. Joseph Breen, Project Officer. This report was prepared by Mr. Jon Onstot with assistance from Mr. Randall E. Ayling and Dr. John S. Stanley, MRI Work Assignment Leader.

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EXECUTIVE SUMMARY

The National Human Adipose Tissue Survey (NHATS) provides the EPA Office of Toxic Substances with a unique mechanism for establishing exposure of the general U.S. population to toxic compounds. This monitoring program has been used primarily for establishing exposure trends for organochlorine pesticides and PCBs. The adipose specimens collected in fiscal year 1982 (FY82) were analyzed as composites for general volatile and semivolatile organic compounds as part of an effort to expand the use and capabilities of the NHATS program. This effort was undertaken as a means to detect potentially toxic compounds that might be entering the environment.

The FY82 samples were composited into 46 samples and were analyzed by high resolution gas chromatography/mass spectrometry (HRGC/MS). Quantitative data were reported for a specific list of volatile and semivolatile organic compounds. The response to these compounds is a fraction of the total HRGC/MS response for each of the composites. Many of the peaks in the HRGC/MS chromatograms remain unidentified. As part of the effort to document human exposure to toxic chemicals, it is necessary to identify as many of these responses as possible.

A method for the automatic identification of unknown HRGC/MS peaks was developed and applied to the volatile and semivolatile datafiles. The files were analyzed in three groups: volatiles, and semivolatiles from two fractions collected from Florisil cleanup (6% diethyl ether/hexane, and 15/50% diethyl ether/hexane).

The method consisted of the following steps: automatic identification of unknown spectra via comparisons to reference mass spectra, transfer of the results to a microcomputer for additional processing, compilation of the transferred data into a spreadsheet program, and generation of compound identification tables from the spreadsheet. A computer program, called ACORN, was written to perform the automatic identification step.

Application of this method to the three sets of data resulted in the identification of 121 compounds in the volatile samples, 81 compounds in the 6% Florisil semivolatiles, and 96 compounds in the 15/50% Florisil semivolatiles. These compounds are in addition to the compounds identified and quantitated in the target compound search previously reported (Stanley 1986a, Stanley 1986b, Stanley 1986c). Identified compounds were grouped into 18 chemical classes for the volatiles, 22 classes for the 6% Florisil semivolatiles, and 21 classes for the 15/50% Florisil semivolatiles. Compound classes included saturated and unsaturated hydrocarbons, aldehydes, ketones, steroids, heterocyclic compounds, drugs, aliphatic and phthalate esters, phenols, halocarbons, and methyl-substituted organosiloxanes.

An additional 99 spectra remained unidentified in the volatile samples, and 258 and 343 spectra in the 6% and 15/50% Florisil semivolatiles, respectively.

I. INTRODUCTION

The National Human Adipose Tissue Survey (NHATS) is the main operative program of the National Human Monitoring Program (NHMP). The NHMP was first established by the U.S. Public Health Service in 1967 and was subsequently transferred to the U.S. Environmental Protection Agency in 1970. During 1979 the program was transferred within EPA to the Exposure Evaluation Division (EED) of the Office of Toxic Substances (OTS).

NHATS is an annual program to collect a nationwide sample of adipose tissue specimens and to chemically analyze them for the presence of toxic compounds. The objective of the NHATS program is to detect the level and prevalences of the compounds in the general population. The NHATS data are used to address part of OTS's mandate under the Toxic Substances Control Act (TSCA) to assess chemical risk to the U.S. population. The specimens are collected from autopsied cadavers and surgical patients according to a statistical survey design (Lucas, Pierson, Myers, Handy 1981). The survey design ensures that specified geographical regions and demographic categories are appropriately represented to permit valid and precise estimates of baseline levels, time trends, and comparisons across subpopulations. Historically, organochlorine pesticides and PCB residues have been selected for evaluation.

A. Broad Scan Analysis Strategy

EPA/OTS has recognized the need to provide a more comprehensive assessment of the toxic substances that accumulate in adipose tissue. An aggressive strategy to assess TSCA-related substances that persist in the adipose tissue of the general U.S. population has been developed by EED. The NHATS specimens collected during fiscal year 1982 (FY82) were selected for a broad scan analysis of volatile and semivolatile organic TSCA-related chemicals (Mack, Stanley 1984).

The initiative to achieve a more comprehensive assessment necessitated either the development of new methods or the modification of the existing analytical procedures, specifically high resolution gas chromatography/mass spectrometry (HRGC/MS). Data on organochlorine pesticides and PCBs reported for the NHATS specimens up to the FY82 collection are based on packed column gas chromatography/electron capture detector (PGC/ECD) analysis.

Under a previous work assignment program for EPA/OTS, Midwest Research Institute (MRI) conducted the analysis of human adipose tissue as composites for a specific list of organic compounds (Stanley 1986a, Stanley 1986b, Stanley 1986c, Stanley 1986d). Forty-six composites from the NHATS FY82 collection period were analyzed for volatile and semivolatile organic compounds by HRGC/MS. Although the broad scan analysis approach for a specific list of compounds provided EPA/OTS with an expanded list of potentially toxic compounds in adipose tissue, a number of peaks observed in the HRGC/MS reconstructed ion chromatograms (RIC) were not identified.

Preliminary procedures were developed to automatically characterize the unidentified peaks, and a pilot study of 10 samples was conducted to test the procedures. Results of this pilot study proved encouraging enough to launch the study of the entire volatile and semivolatile sample set.

B. Work Assignment Objectives

The work assignment had three major objectives: (1) automatically characterize HRGC/MS chromatographic peaks (i.e., identify compounds by name) via comparison of unknown spectra to NBS mass spectral library reference spectra; (2) compile a comprehensive database of mass spectra observed in the NHATS composite samples; and (3) determine the frequency with which each compound or unidentified mass spectrum was observed in the sample set.

C. Significance

At the present time, the NHATS program is limited to the screening of a predetermined list of toxic substances. The philosophy of using a relatively small list of target compounds is common in programs requiring GC/MS analysis of large numbers of samples. The advantages of this technique are numerous. Acquisition of full scan HRGC/MS data for target compound analysis is standardized and does not usually require extensive setup time. Operating conditions for target compound analysis may be optimized for a particular sample type and anticipated concentration range, resulting in good sensitivity for most compounds. The post-acquisition target analyte identification and quantitation step is relatively fast, usually requiring less than 30 s per compound. Finally, both acquisition and quantitation may be easily automated.

However, a major drawback to the target compound approach is that nontarget HRGC/MS peaks do not enter into the analysis process. As a result, the overall significance of a sample or population of samples may be incorrectly interpreted. The situation is unfortunate because the mass spectral information necessary for unknown compound identification is available from datafiles acquired for target compound analysis.

The reason why this information is not typically used for unknown peak identification is straightforward: the technology to automatically process mass spectral information on this scale has not kept pace with the technology to acquire it. As a result, acquisition may take minutes, while a complete post-acquisition analysis of unknown constituents might require hours, days, or even months, depending on the amount of information contained in the data. Thus, target compound analysis may be regarded merely as a simplification of the larger, more difficult goal of complete characterization of real samples.

This report describes a method for the automatic identification of HRGC/MS chromatographic peaks in the data from the volatile and semivolatile organic analysis of composite adipose tissue samples. The method consists of the following steps: automatic identification of unknown spectra via comparisons to reference mass spectra; transfer of the results to a microcomputer for additional processing; compilation of the tranferred data into a spreadsheet program; and generation of compound identification tables from the spreadsheet. A computer program, called ACORN, was written to perform the automatic peak identification step.

Application of the method to the three sets of data resulted in the identification of 121 compounds in the volatile samples, 81 compounds in the 6% Florisil semivolatiles, and 96 compounds in the 15/50% Florisil semivolatiles. An additional 99 spectra remained unidentified in the volatile samples, and 258 and 343 spectra in the 6% and 15/50% Florisil semivolatiles, respectively.

D. Organization of this Report

Following this introductory section, Section II presents recommendations for pursuing future activities in characterizing unidentified HRGC/MS peaks and developing a mass spectral database for adipose tissue. Section III is the experimental section and presents a description of the identification method and criteria incorporated in the computer-controlled search to characterize the HRGC/MS data. The results from the application of this automated search program are presented in Section IV. Section V discusses the technical difficulties that were encountered using this approach to characterize the volatile and semivolatile HRGC/MS data. Pertinent references are cited in Section VI. Supplementary tables and a listing of ACORN, the peak identification computer program, are provided in Volume II (Appendices).

II. RECOMMENDATIONS

Recommendations for further activities in the area of unidentified peaks may be divided into three major areas: refinement of the identification procedure; confirmation of compounds identified in this study; and further investigation of the remaining unidentified peaks.

A. Refinements to the Identification Method

A number of refinements could be made to the identification procedure to improve reliability and execution speed. Reliability could be improved by more fully utilizing the available retention time information. For example, the work in this study relied on a single reference compound for the calculation of the relative retention times (RRTs) of the unknown peaks. However, procedures could be developed to include retention information for surrogate compounds, target compounds known to be present in samples, or commonly observed background peaks. This could even be extended to include the unidentified peaks themselves. For example, analysis of a file might begin with the unknown peak closest to the internal standard. If the unknown peak could be positively identified from the reference library, it could then be used as the reference for the unknown peak adjacent to it, and so on until all peaks in the file are analyzed. Differences in retention time between unknown and reference are minimized using this scheme, thus improving the accuracy of the retention time test.

A major limitation of the Incos-based library search routine is that no attempt is made to judge the quality of the unknown spectrum. The Incos data system makes the assumption that spectra submitted to the library routines are of high quality. Unfortunately, this assumption may not be valid for spectra submitted in an automatic procedure. Thus, this requires significant interaction through manual review of the data. It would be useful if a

test could be performed on the unknown spectrum which would provide a quantitative measure of its quality, such as the percentage of masses rising above the surrounding signal-to-noise level, whether any masses might belong to coeluting peaks or background, or whether a molecular ion is present. A weighted quality index might then be assigned which could be used to assess the validity of subsequent library searches during automatic processing.

Other possible refinements to the identification procedure might include translation of the ACORN program code to FORTRAN instead of using the macro or "procedural" language of the Incos data system and addition of more information to the ACORN summary report, such as RRT and mass spectrum quality index values (described above) for each peak. Programs could also be written to automatically perform a number of bookkeeping activities on the seed library that are presently done by an operator at a video terminal. Finally, the transfer of data from the Incos to the microcomputer could be streamlined with additional programming. These refinements would require an additional level of effort which would probably not be recovered through increased efficiency on a small peak identification project. For large scale peak identification projects, however, the resulting efficiency would justify the additional expense.

B. Compound Confirmation

It is strongly recommended that some type of confirmatory work be performed for compounds which were tentatively identified in this study. A significant number of identified compounds could not be traced to a specific isomer. In other cases, peaks could not be assigned to specific compounds within certain chemical classes due to the similarity of mass spectra within the class. Examples of such classes were the homologous series of hydrocarbons, phthalates, isomers of chlorinated compounds, steroids, etc. Ambiguities might be resolved by analysis of standard mixtures using HRGC/MS parameters identical to those used in the original target compound analysis.

C. Additional Investigation of Remaining Unknown Peaks

Many of the HRGC/MS chromatographic peaks analyzed in this study remain unidentified for two main reasons. First, many of the unidentifiable spectra were unsuitable for interpretation purposes even after computerized enhancement was employed. This was the major cause of peaks not being identified in this study. Secondly, the finite nature of the NBS library prevented some spectra from being identified in those cases when the corresponding compound simply was not represented in the library. Despite these difficulties, additional identifications may be possible through analysis of samples using optimized HRGC/MS acquisition parameters, additional mass spectral interpretation programs, or high resolution mass spectrometry.

1. Optimization of HRGC/MS Acquisition Parameters

Improving the quality of the unknown spectra could be accomplished by the reanalysis of a subset of the samples using operating conditions more suitable for unknown peak identification. For instance, using a slow GC program rate ($\sim$ 2°C/min) would help separate peaks that coeluted in the original

analyses, thereby improving the quality of the mass spectra. Longer GC columns could be used, and in the case of the volatile samples a wide bore "Megabore" capillary column might improve separation as well as reduce overloading. A mass scanning range more appropriate to mass spectral interpretation of unknowns could be used for the semivolatiles. Finally, samples could be analyzed at various detection sensitivity settings in order to compensate for differences in unknown compound concentration levels. The improved spectra could then be resubmitted to the ACORN program. It is believed that a significant number of unknown spectra could be identified from this procedure alone.

2. Other Mass Spectral Interpretation Programs and Databases

It is suspected that several peaks in this study were not identified because the corresponding reference spectrum was not present in the NBS library. In such cases, the use of a different mass spectral library might prove successful. One example of a commercially available library is the Wiley Registry of Mass Spectra, containing approximately 120,000 reference spectra on a single compact disk (CD) for use with an IBM-PC. A similar alternative is to submit unidentified spectra of off-site mass spectral interpretation services, such as the Self-Training Interpretive Retrieveal System (STIRS) and Probability Based Matching (PBM) programs available from Cornell University (Kwok, Ventkatarughaver, McLafferty 1973; McLafferty, Hertel, Villwock 1974; Martinsen, Song 1985). A disadvantage to both of these approaches is that a significant effort would be required to convert the large number of remaining unknown spectra to a format compatible with the other data systems.

3. High Resolution GC/High Resolution MS

Additional information could be gained by reanalysis of a subset of the samples using high resolution GC/high resolution MS (HRGC/HRMS). HRMS provides accurate mass information for ions observed in mass spectra. Mass assignments with an accuracy of approximately 5 millimass units (mmu) are achievable for broad scan capillary GC analysis in high resolution mode. Accurate mass values are primarily used to calculate possible elemental formulas for the molecular and fragmentation ions. This information could be used both to confirm the NBS-derived compound assignments and to provide additional information concerning unidentified peaks.

4. Chemical Ionization

Additional information could also be gained from reanalysis using chemical ionization GC/MS. This technique typically produces a stronger signal in the molecular ion than electron impact ionization (EI). Thus, chemical ionization could provide confirmation for a number of compounds which have similar EI spectra, but different molecular weights. An example is the class of straight-chain hydrocarbons, which exhibit nearly identical spectra in the low mass range and which do not usually produce molecular ions in EI.

5. Additional Manual Interpretation

Most of the manual work performed in this study involved reviewing the results of the automatic peak identification procedure. However, additional interpretation could be manually performed on the remaining unidentified peaks. Manual interpretation could potentially provide information not readily available from a spectral matching approach, such as compound class, functional groups and molecular weight.

D. Further Investigations

The results of this study should be examined for significance to further efforts involving the screening of adipose tissue. This would include determining the source, concentration, exposure and level of toxicity of the identified compounds.

III. EXPERIMENTAL PROCEDURE

This section describes the steps involved in the peak identification procedure and their application to the FY82 data. A brief overview of the identification method is provided, followed by a discussion of ACORN, the computer program written to automatically perform the identification step. Various aspects of the computer program as they related to the identification process are discussed. Finally, the application of the identification method to the FY82 data is described.

A. Description of Identification Method

A general method for the identification was devised which consisted of three major steps. The first step involved the selection of peaks to be analyzed. This was accomplished through a combination of manual peak selection and use of the automatic peak selection routine provided in the CHRO program of the Incos data system. A first-pass peak selection was performed using CHRO. The results of the selection were then manually reviewed. Manual review of the automatic peak selection procedure was necessary because the program occasionally had difficulty determining the correct apex of peaks located on the shoulder of others peaks. The program also failed to properly select very broad peaks.

The second step was the identification procedure itself. A computer program, ACORN, was written which performed the identification procedure automatically. The program was designed to operate on a single file at a time, allowing an opportunity for a manual review of the results before proceeding to the next file.

The third step of the method involved the transfer of the results of the identification program to a microcomputer for further data processing. It was necessary to perform this additional data processing on another computer because the Incos data system did not have the software necessary to perform the desired tasks. An Apple Macintosh with a 20-megabyte Winchester hard disk drive was used for both the transfer step and the additional data processing. The transfer was relatively straightforward since the Macintosh also functioned as the display terminal for the Incos data system via terminal emulation software. Since all the transferrable information was in text format, the transfer process simply involved instructing the Incos to display the information on the Macintosh screen while in terminal emulation mode, and then instructing the Macintosh to "capture" or store the displayed data to its own disk. The transferred text was then reformatted so that it could be loaded into a spreadsheet program.

The final step of the method, compilation into the spreadsheet program and generation of data tables, was relatively straightforward. Microsoft EXCEL for the Macintosh was the spreadsheet program chosen for this study. Three main spreadsheets were produced from the FY82 data, each spreadsheet consisting of compound information from one of the three types of analysis. Each spreadsheet was arranged as a two-dimensional array of samples vs. compounds identified in the samples. Once the main spreadsheets were compiled, summary tables were generated which listed such information as compound name, CAS registry number, compound formula, relative retention time (RRT), as well as frequency of occurrence within certain age groups and geographical regions.

B. Description of ACORN

The most essential element of the method was the computer program which automatically performed the compound identifications. The program, called ACORN, was written using a combination of FORTRAN and the "procedural" or macro language of the Finnigan/Incos data system. ACORN was designed to perform a "two-tiered" forward library search on each HRGC peak in a datafile, as shown in the program flowchart in Figure 1. Under this scheme, each spectrum in a datafile was first compared against a special mass spectral library of dynamic length, hereafter referred to as the "seed" library. The library search produced a list of possible candidates based on comparison of two similarity index values, FIT and PURITY, to preset threshold values. Candidate spectra with similarity index values above the threshold were further screened using an RRT test.

If a suitable match could not be found in the seed library, a second library search was conducted using the standard NBS library as the reference library. Since no RRT data are provided in the NBS library, selection of the best reference candidate was determined solely by comparing FIT and PURITY values to preset threshold values. If a suitable match was found in the NBS library, the NBS spectrum was appended to the seed library. If a match could not be found in either the seed or the NBS library, the unknown spectrum itself was appended to the seed library and assigned the name "Unidentified Peak." Since spectra were added to the seed library only on the precondition that they had not previously been observed in the data set, the seed library served as a comprehensive database of unique spectra observed in a given data set.

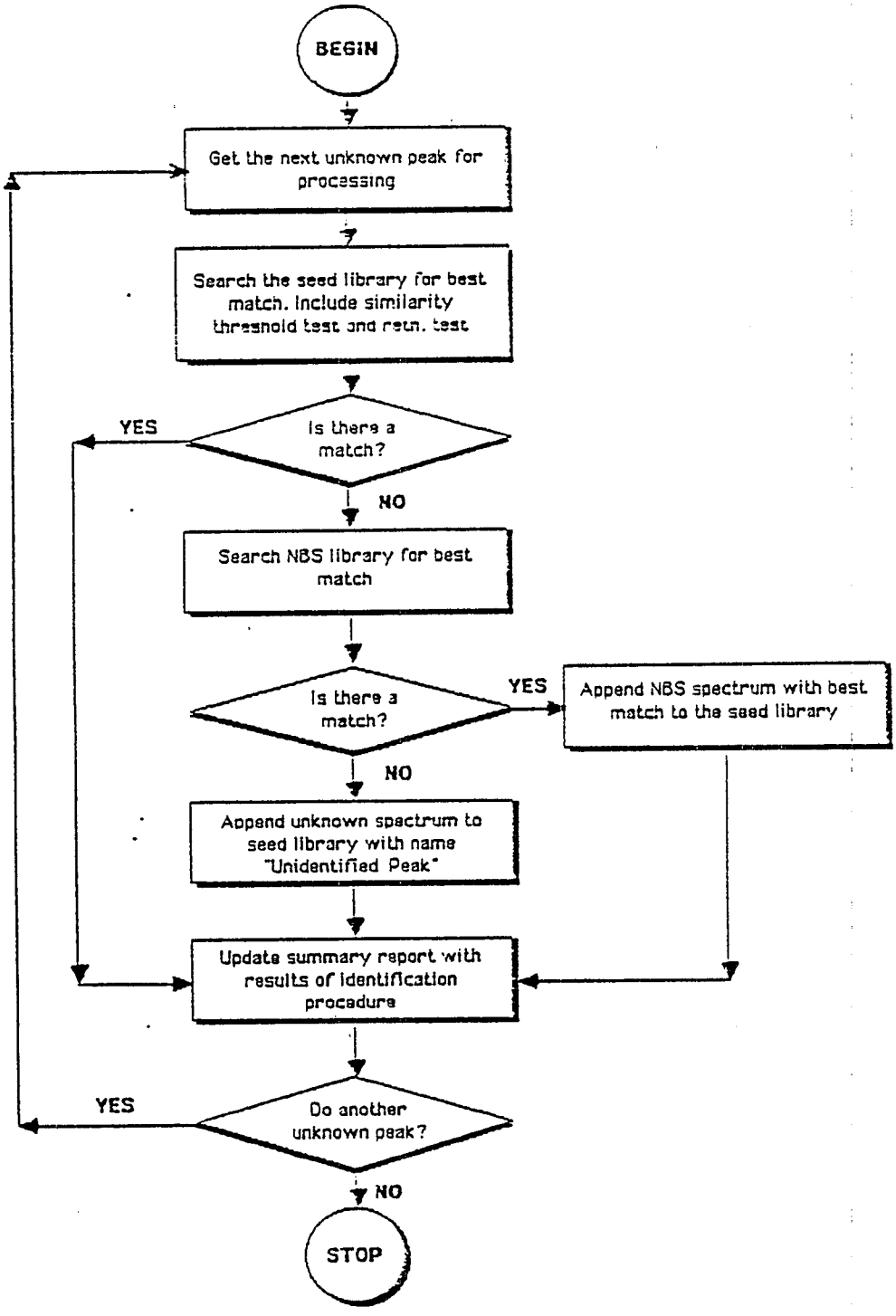

Figure 1. Flowchart of ACORN peak identification program.

C. Library Search Criteria

As stated previously, a two-tiered library searching scheme was applied in ACORN. This approach was used for the following reasons. First, it provided the basis for the design of the automatic compilation of the "seed" library. Second, ACORN execution time was reduced. The seed libraries compiled from the data in this report contained 249, 432, and 537 entries for the volatile, 6% and 15/50% Florisil semivolatile samples, respectively. The version of the NBS library used in this study contained 42,222 reference spectra (Heller, Milne 1983). Since the time required to perform a library search is roughly proportional to the number of spectra in the reference library, a typical search using any of the seed libraries required only a fraction of the time necessary to perform the same search against the NBS library. And third, the two-library approach provided a simple means of implementing the RRT test.

Both the seed and NBS library searches were performed using the standard Incos library search program, called LIBR. When a library search of an unknown spectrum is performed, LIBR calculates two values for each reference spectrum which relate to its similarity to the unknown spectrum. These values, called FIT and PURITY, range from 0 to 1000. A value of 0 for either FIT or PURITY indicates no similarity, while a value of 1000 indicates maximum similarity. FIT and PURITY values may be negatively affected by such conditions as the presence of background contamination or coeluting peaks.

The ACORN program tested minimum FIT and PURITY values to determine whether an unknown spectrum was found in the seed or NBS libraries. Threshold limits were determined by evaluating the result of using various values when applied to library searches of a set of test spectra. It was found that searches of the seed library could be performed reliably using PURITY and FIT values of 300 and 800 for the volatile samples, and 600 and 800 for the semivolatile samples. NBS library searches required PURITY and FIT values of 800 and 900 for both volatiles and semivolatiles.

Threshold values were relatively relaxed in the seed library search because the additional RRT test tended to reduce the number of false positive identifications. The NBS search, with no RRT test, required more stringent threshold values in order to assure a high degree of confidence in compound identification. Volatile samples required different threshold values than the semivolatiles primarily because of differences in operating conditions. A discussion of these differences is presented in Section V.

D. Retention Time Test

A major limitation of the standard Incos library search routine was that it often provided more than one acceptable candidate from the available choices. This situation often arose for isomers of a single compound, such as the various PCBs, or for a family of structurally related compounds whose spectra were dominated by fragmentation ions characteristic for the common molecular skeleton. Examples of this type were the various straight-chain hydrocarbon series, fatty acid esters, and phthalates. In such cases, the library search routine was unable to reliably select a match from the various

candidate spectra because each of them was equally valid from a spectral point of view. An example of multiple candidate reference spectra is shown in Figure 2. In this example, the results of an NBS library search conducted on an unknown peak are displayed. The first section of the results output shows various information about the sample itself, followed by a table of the three best candidate spectra from the NBS library and their FIT and PURITY values. Following the table, a graphic comparison of the unknown spectrum and the three candidates is given. As can be seen from the FIT and PURITY values and the graphic comparisons, all three candidates are very similar to the unknown spectrum, and further selection using the available data is impossible.

In order to differentiate the numerous observed compounds with similar spectra, an RRT test was employed to take advantage of the fact that compounds with similar mass spectra had unique retention times. The test was performed immediately after the seed library search, utilizing information provided by the search. This test compared the unknown GC peak's RRT to the RRT values of each of the candidate spectra. A final candidate was chosen from entries passing the previous tests by selecting the entry with the RRT closest to the unknown. A match was considered successful if the final candidate passed the library similarity test, had the closest RRT to the unknown of all candidates passing the library test, and whose predicted retention time (calculated as $RRT_{candidate} \times RT_{internal\ standard}$ fell within a window ± 15 s from the unknown.

E. Manual Review of ACORN Results

Upon completion of each sample analysis using ACORN, a summary report was produced which listed information about the search results of each analyzed peak. An example of an ACORN summary report is shown in Figure 3. In this example, 40 unknown peaks were analyzed, as indicated in the Peak No. column. FIT and PURITY values for best match in the library in which each peak was found are also given. For those peaks which were found in the NBS library, the corresponding NBS library entry number is provided. The column titled "CURRENT ENTRY" shows either the seed library entry number which was the best match to the unknown spectrum or the seed entry number to which an NBS or unknown spectrum was appended.

The results of the program were then manually reviewed. The first step of the review consisted of checking the ACORN summary report to verify that the program had operated properly. Next, each mass spectrum appended to the seed library was checked to ensure that it was indeed a newly observed spectrum. This was accomplished by manually examining the NBS search results, such as shown in Figure 2, for each appended spectrum. As can be seen in the figure, this output provides a ranking of the three best candidate reference spectra in addition to the unknown spectrum. The ACORN program always selected the first ranked candidate spectrum for addition to the seed library. However, if it was determined from manual review that other candidate spectra were equally valid choices, the name of the compound was changed to reflect the uncertainty of the selection. For example, the name of the compound associated with the spectrum shown in Figure 2 was changed to "C_5 substituted naphthalene." Finally, the RRT, PURITY, and FIT values were checked for all

```
Library Search                          Data: 7901D19R3 # 623      Base m/z:   161
04/19/84 11:52:00 + 13:30               Cali: CALD19R1 #   3       RIC:       8943.
Sample: 7901-8-046 6% 1-PA-SVO-0-14 1UL INJ (2UG D-10 ADDED)
Conds.: -1700EMV 70EV 1MA DB5-30M 60-2H-310-10/ 45SEC. SPLT.
Enhanced (S 15B 1N 0T)

38754 spectra in LIBRARYNB searched for maximum PURITY
   99 matched at least 6 of the 16 largest peaks in the unknown

Rank In.      Name
1 16041 1H-CYCLOPROPA[A]NAPHTHALENE, 1A,2,3,5,6,7,7A,7B-OCTAHYDRO-1,1,7,7A-+
2 16033 NAPHTHALENE, 1,2,3,5,6,7,8,8A-OCTAHYDRO-1,8A-DIMETHYL-7-(1-METHYLET+
3 16055 1H-CYCLOPROP[E]AZULENE, DECAHYDRO-1,1,7-TRIMETHYL-4-METHYLENE-, (1A+

Rank  Formula    M. Wt  B. Pk   Purity   Fit   RFit
1     C15. H24     204    161      862   964    873
2     C15. H24     204    161      851   970    859
3     C15. H24     204    161      836   947    842
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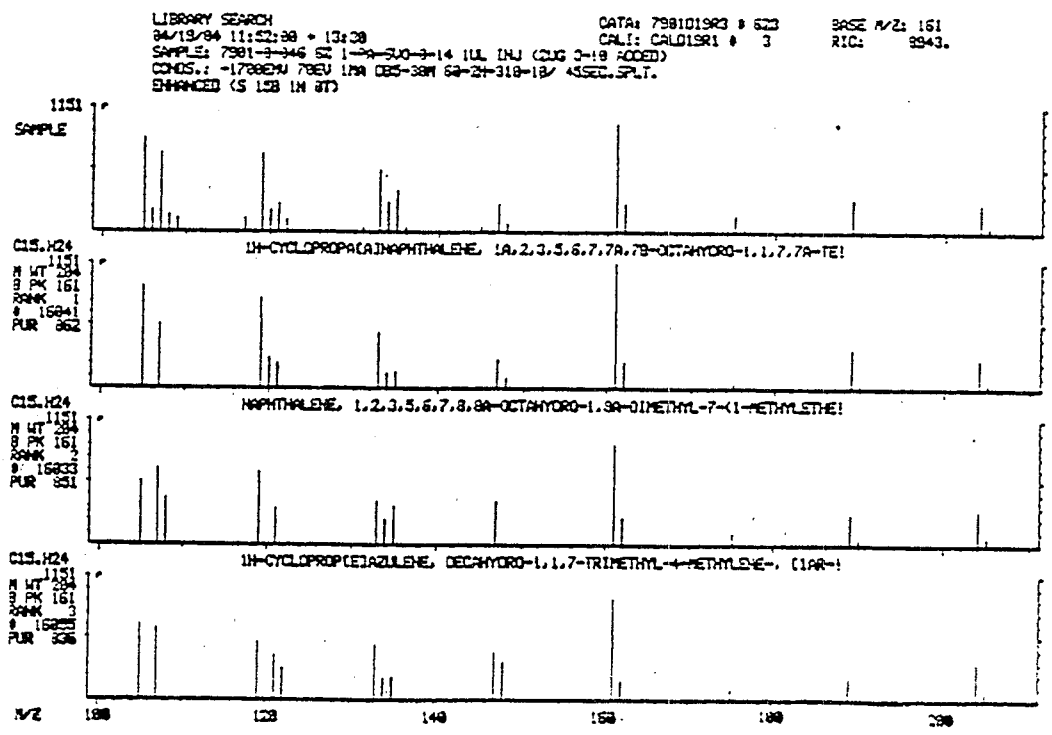

Figure 2. Library search results of unknown peak with multiple candidate compound identifications.

ACORN LIBRARY SEARCH RESULTS FILENAME: 7901D23R5

PEAK NO.	SCAN NO.	PEAKS /SCAN	BEST FIT	BEST PURITY	BEST NBS ENTRY	LIBRARY CHOICE	CURRENT ENTRY
1	254	7	906	622	5852	NBS	686
2	261	9	933	790	6202	NBS	687
3	305	14	893	565	9588	UNKN	688
4	334	13	897	891		SEED	121
5	348	19	995	984		SEED	121
6	357	15	962	959		SEED	123
7	360	15	954	950		SEED	123
8	368	17	883	870		SEED	124
9	373	26	973	942		SEED	125
10	380	6	947	947		SEED	126
11	384	10	729	345	21473	UNKN	689
12	399	10	990	807	5692	NBS	690
13	417	7	790	377	31109	UNKN	691
14	428	8	995	794	1930	NBS	692
15	441	4	996	913	1391	NBS	693
16	461	9	995	872	4155	NBS	694
17	476	12	995	779		SEED	694
18	486	10	946	620	11868	NBS	695
19	490	10	866	617	15161	UNKN	696
20	525	17	817	364	7014	UNKN	697
21	684	15	1000	800		SEED	14
22	807	30	998	786		SEED	1
23	845	9	906	906	*-313	NBS	698
24	896	26	947	907		SEED	166
25	922	9	676	449	10926	UNKN	699
26	948	7	908	594	3425	UNKN	700
27	994	9	702	545	*-327	UNKN	701
28	1043	26	890	816	*-291	UNKN	702
29	1069	10	781	743	31228	UNKN	703
30	1090	8	553	528	30302	UNKN	704
31	1104	38	958	860	24638	NBS	705
32	1171	39	971	926		SEED	175
33	1232	32	957	845		SEED	176
34	1268	25	772	510	*-270	UNKN	706
35	1308	27	700	491	*-270	UNKN	707
36	1314	79	872	546		SEED	180
37	1323	54	913	638		SEED	181
38	1458	59	930	778	*-263	NBS	708
39	1465	18	655	537	*-252	UNKN	709
40	1508	19	523	370	30560	UNKN	710

Figure 3. Example of an ACORN summary report. The columns titled "Best Fit" and "Best Purity" refer to results of the seed search if the peak was identified from the seed library or to results of the NBS search if it was not identified from the seed library. The column titled "Library Choice" indicates the final choice of ACORN for the unknown peak.

entries which were identified from the seed library. Entries with library PURITY and FIT values near the threshold limits were checked by visually comparing the search results to the actual spectrum from the sample.

RRT values were checked by superimposing a hardcopy of the sample's reconstructed ion current (RIC) profile over a "master RIC" which was marked with the precise RRT of every seed library entry. The superimposition of RICs proved to be a very useful and reliable technique. It was a simple matter to line up commonly occurring major peaks and then compare each sample peak with its corresponding seed entry peak on the master RIC. In most cases, the sample peak was exactly superimposed on its corresponding reference peak. Examples of a "test RIC" and a "master RIC" are shown in Figure 4. The RRT test within ACORN itself precluded the possibility of more than minor differences between sample and reference RRT. However, the program occasionally erred if two or more compounds with identical or very similar spectra were located within a retention window which was narrower than the window of the RRT test (± 15 s) in ACORN. Manual comparison to the master RIC as described above was usually effective in resolving these difficult cases. It was possible for an experienced operator to manually review a datafile containing 60 to 80 peaks in about an hour.

F. Application of the Identification Method to FY82 NHATS Data Set

The data set utilized for this study consisted of composited human adipose tissue specimens prepared from the NHATS repository which were originally analyzed as part of a broad scan study. The composite samples were originally analyzed by HRGC/MS for volatiles and semivolatile target compounds during the period from April 1984 to July 1984 (Stanley 1986b, Stanley 1986c).

The composites consisted of 46 volatiles, 44 semivolatiles from the 6% Florisil cleanup fraction, and 46 semivolatiles from the 15/50% Florisil cleanup fraction. Within each of these categories, there were 12, 17, and 17 samples in the 0-14, 15-44, and 45+ age groups for the volatile and 15/50% Florisil semivolatile datafiles, and 12, 15, and 17 samples in the 0-14, 15-44, and 45+ age groups for the 6% Florisil semivolatile datafile.

Each data set was treated separately throughout the peak identification procedure. Separate seed libraries were maintained for each group of samples. The volatile data set was analyzed entirely before proceeding to the semivolatile samples. Semivolatile samples were analyzed in order of age group; i.e., the 0-14 yr samples for both 6% and 15/50% samples were analyzed prior to the 15-44 yr samples, and the 45+ samples were analyzed last. It has been observed that the number of extractable components in adipose tissue is dependent upon the age of the individual from which the sample was taken. The analysis sequence described above was used so that analysis could proceed from samples with relatively few unknown peaks to samples with large numbers of unknown peaks. Examples of the differences between samples from various age groups from the volatile, 6%, and 15/50% Florisil semivolatile composites are shown in Figures 5 through 7, respectively.

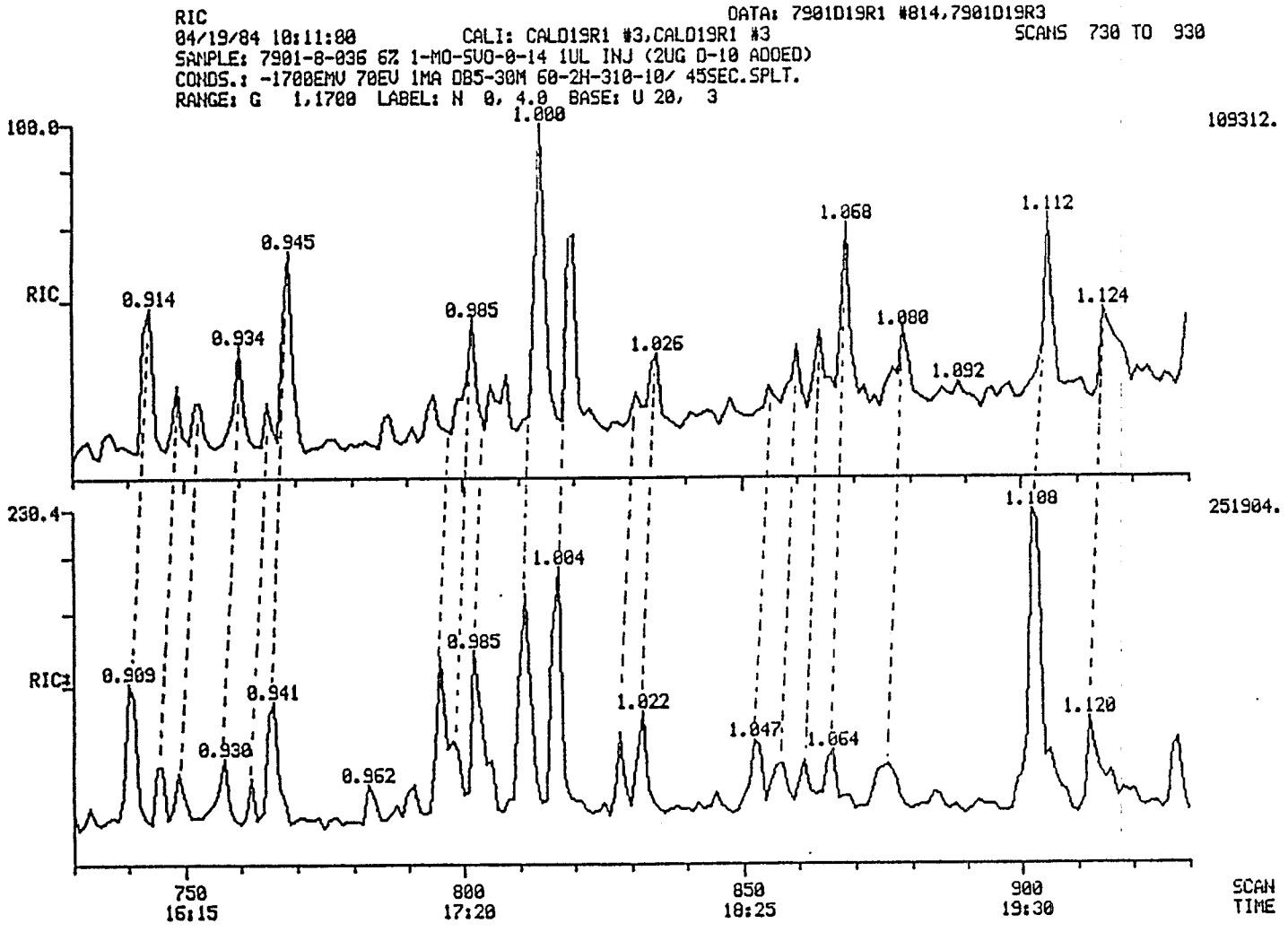

Figure 4. Example of the manual review of RRT values using a "Master RIC." In this example, the upper RIC is the master and the lower RIC is being reviewed. If a peak is observed in the test RIC which is not on the master RIC, its location and seed entry number are recorded on the master in case it is observed in the future.

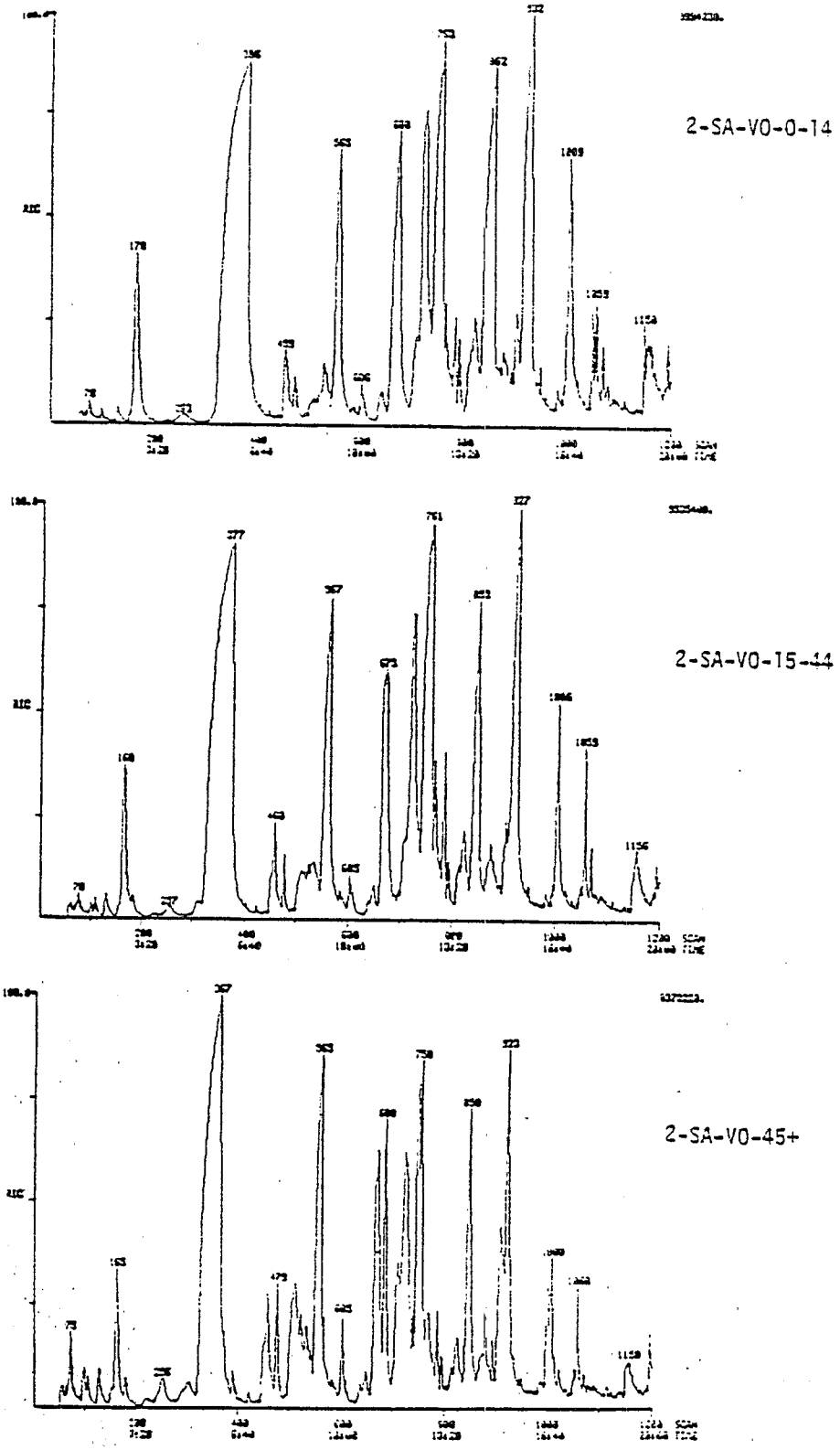

Figure 5. Reconstructed ion chromatogram (RIC) of volatile composites from the 0-14, 15-44, and 45+ age groups from the South Atlantic (SA) census division.

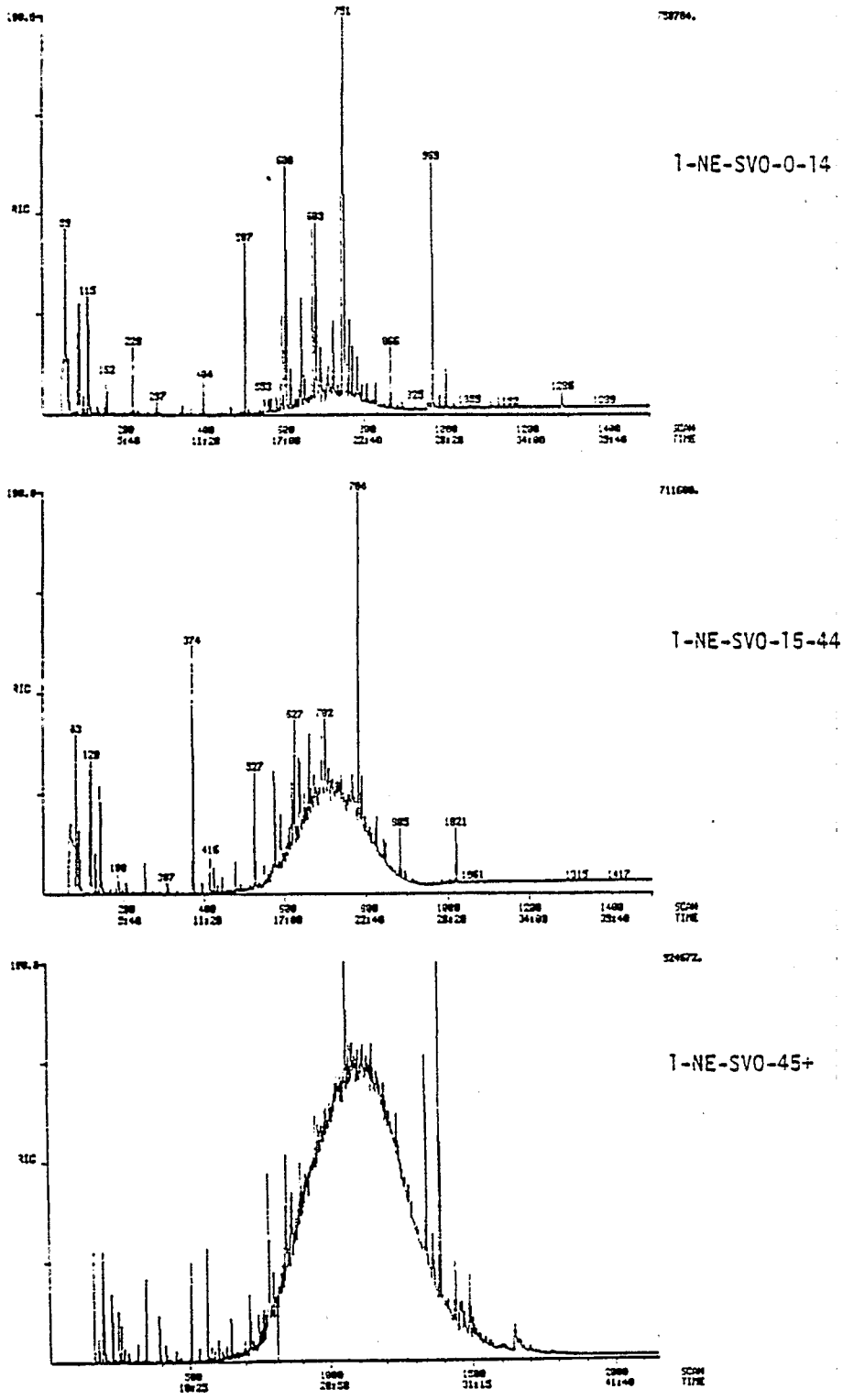

Figure 6. Reconstructed ion chromatogram (RIC) of 6% Florisil semivolatile composites for the 0-14, 15-44, and 45+ age groups from the New England (NE) census division.

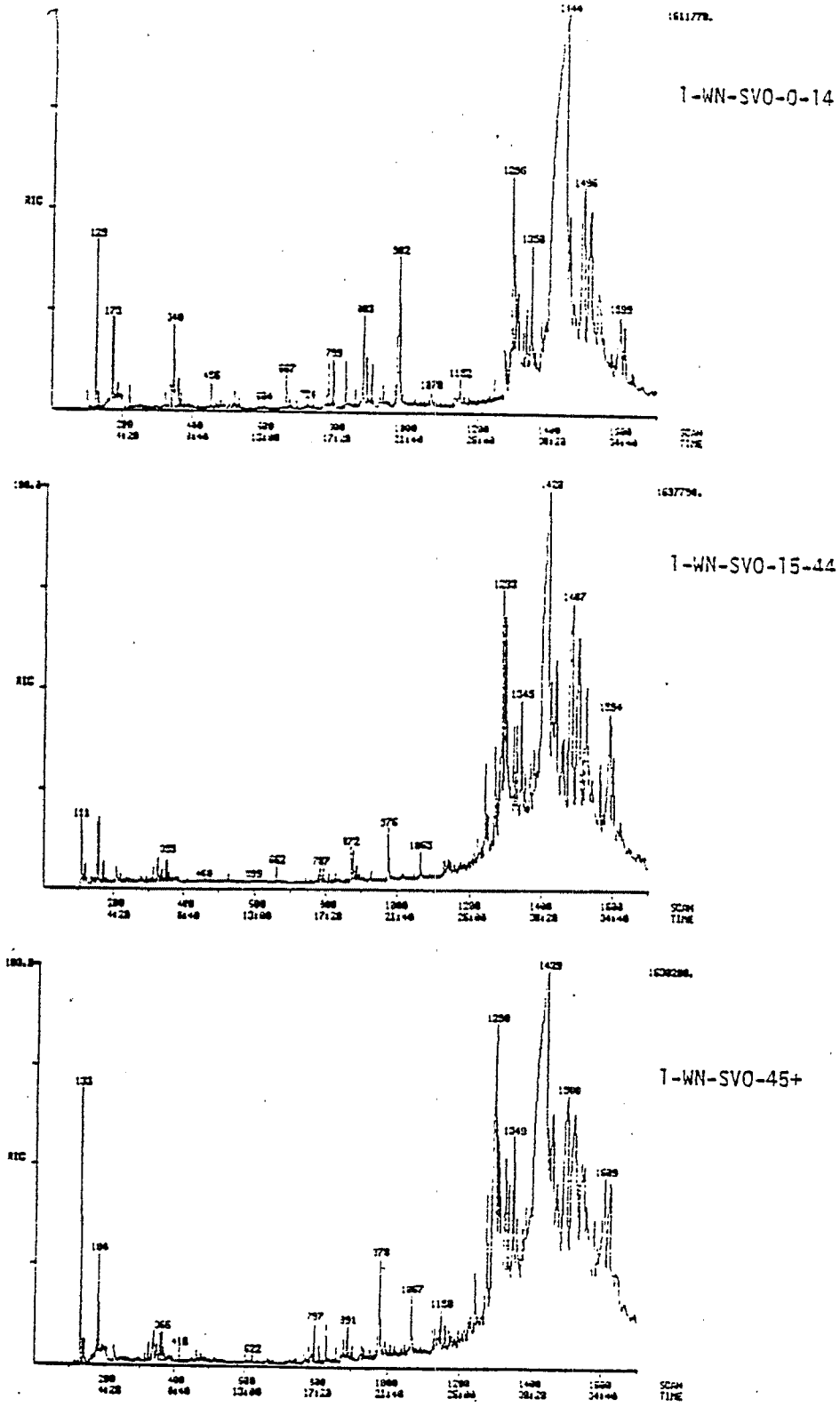

Figure 7. Reconstructed ion chromatogram (RIC) of 15/50% Florisil semivolatile composites for the 0-14, 15-44, and 45+ age groups from the West North Central (WN) census division.

IV. RESULTS

Application of the peak identification procedure to the FY82 composites as described above resulted in the following tables of results. Twelve tables (Tables 1 through 12) are provided in this report which list all NBS identified compounds from the three composite data sets as well as information regarding peaks still unidentified. An additional six tables (Tables A-1 to A-6) are provided in Appendix A (Volume II) to this report which include more detailed information regarding the incidence of occurrence of peaks in the three data sets.

Tables 1 through 3 present the compounds identified via comparison to NBS reference spectra for the volatile, 6% Florisil semivolatile, and 15/50% Florisil semivolatile samples, respectively. Each table consists of the following information in columnar form. The first column shows an index number, which is simply a sequential numbering of the compounds listed in the table. The index number is not related to any other numbering order in previous reports. The Compound Class column indicates the chemical class to which a compound belongs. Chemical class designations were determined by manual inspection of the compound names. The Compound Name, Formula, and CAS No. columns are derived from the NBS library resident on the Incos data system. In most cases, the names are unaltered from the name in the NBS library. In some cases, however, the peak identification procedure was unable to accurately specify a positional isomer, and the positional portion of the NBS name was either removed or placed in parentheses. For compounds with positional designations in parentheses, the corresponding CAS number refers to the given isomer. The remaining columns show the frequency of occurrence of the listed compounds within the three tested age groups: 0-14, 15-44, and 45+ yr.

Tables 4 through 6 show the same information as Tables 1 through 3, with the exception that frequency of occurrence data are arranged according to census region [North Central (NC); Northeast (NE), South (S), and West (W)]. Information regarding age groups is not given. The three tables represent data for the volatile, 6%, and 15/50% Florisil fractions, respectively.

Tables 7 through 9 show the frequency of occurrence data for peaks which ACORN was unable to identify from the NBS library. As with the previous sets of tables, Tables 7 through 9 represent data compiled from the volatile, 6%, and 15/50% Florisil fractions, respectively. The list of entries is sorted by descending frequency of occurrence. Occurrence data are also listed for each census region.

Tables 10 through 12 represent the degree to which the unknown peaks in the FY82 data were identified, and thus may be considered "peak inventories" for the analyzed data. The tables list the number of peaks selected for analysis for each of the composites in this study, the number of peaks identified by ACORN from comparison to the NBS library, the number of peaks which remain unidentified, and the number of compounds identified and quantitated in the target compound search previously reported (Stanley 1986b, Stanley 1986c). This information provides a general guide for the amount of work which remains to be done for complete characterization of the composite samples.

Table 1. Compounds Tentatively Identified in the Volatile Organic Analysis Data Set vs. Frequency/Age Group

Index	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS No. (c)	Number of Occurrences In All Samples	In Each Age Group 0-14	15-44	45+
I.S.	Internal Standard	Bromochloropropane - Internal Standard			46	12	17	17
1	Carbon Dioxide	Carbon dioxide	C.O2	124-38-9	45	12	17	16
2	Alkane	2-Methyl-butane	C5.H12	78-78-4	18	6	6	6
3		Unidentified C5.H10 [Cyclopentane]	C5.H10	287-92-3	7	3	3	1
4		C3 Substituted cyclopropane [Propyl-cyclopropane]	C6.H12	2415-72-7	13	2	7	4
5		C3 Substituted cyclopropane [Propyl-cyclopropane]	C6.H12	2415-72-7	22	3	8	11
6		2,3-Dimethyl-hexane	C8.H18	584-94-1	31	6	14	11
7		1,2-Diethyl-cyclobutane	C8.H16	61141-83-1	3	2	1	0
8		Alkane ≥ C10 [Decane]	C10.H22	124-18-5	16	4	4	8
9		C10 Alkane [2-Methyl-nonane]	C10.H22	871-83-0	9	2	3	4
10		2,2,3,3-Tetramethyl-hexane	C10.H22	13475-81-5	10	1	2	7
11		Sat. alkane ≥ C11 [2-Methyl-decane]	C11.H24	6975-98-0	6	1	5	0
12		Alkyl substituted hexane [Pentyl-cyclohexane]	C11.H22	4292-92-6	1	0	0	1
13		2,2-Dimethyl-decane	C12.H26	17302-37-3	13	4	4	5
14		C13 Alkane [3,3-Dimethyl-undecane]	C13.H28	17312-65-1	1	0	0	1
15		Alkane [6-Ethyl-2-methyl-decane]	C13.H28	62108-21-8	8	2	3	3
16		Alkane [2,6,7-Trimethyl-decane]	C13.H28	62108-25-2	21	3	7	11
17		Alkane ≥ C11 [5-(1-Methylpropyl)-nonane]	C13.H28	62185-54-0	1	0	0	1
18		C13 Alkane [2,2,7-Trimethyl-decane]	C13.H28	62237-99-4	10	2	4	4
19		3,3,8-Trimethyl-decane	C13.H28	62338-16-3	1	0	0	1
20		Alkane [6-Methyl-tridecane]	C14.H30	13287-21-3	4	1	1	2
21	Alkene	C5 Alkane [1-Pentene]	C5.H10	109-67-1	4	1	0	3
22		1-Hexene	C6.H12	592-41-6	15	7	5	3
23		Unidentified C6.H12 [1-Hexene]	C6.H12	592-41-6	24	6	9	9
24		3-Methyl-1,4-heptadiene	C8.H14	1603-01-6	4	0	0	4
25		1,6-Octadiene	C8.H14	3710-41-6	4	3	1	0
26		1,3,6-Octatriene	C8.H12	22038-69-3	10	3	1	6
27		Unidentified C8.H12 [3-Ethylidene-1-methyl-cyclopentene]	C8.H12	62338-00-5	1	0	0	1
28		1-Nonene	C9.H18	124-11-8	8	2	4	2
29		3-Ethyl-2-methyl-1,3-hexadiene	C9.H16	61142-36-7	44	12	17	15
30		C10 Ringed alkene [1,7,7-Trimethyl-bicyclo[2.2.1]hept-2-ene]	C10.H16	464-17-5	44	10	17	17
31		1-Methyl-4-(1-methylethenyl)-cyclohexene	C10.H16	5989-54-8	1	1	0	0
32		7-(1-Methylethylidene)-bicyclo[4.1.0] heptane	C10.H16	53282-47-6	1	0	0	1
33		C11 Alkene [1-Undecene]	C11.H22	821-95-4	8	3	5	0
34		C11 Alkene [1-Ethenyl-2-hexenyl-cyclopropane]	C11.H8	22822-99-7	2	0	0	2
35		Isomer of Undecen-3-yne [5-Undec-3-yne]	C11.H18	74744-31-3	17	4	4	9
36		Isomer of Undecen-3-yne [5-Undec-3-yne]	C11.H18	74744-31-3	31	8	12	11
37	Arene	C2 Alkyl benzene [1,2-Dimethyl-benzene]	C8.H10	95-47-6	41	9	16	16
38		C2 Alkyl benzene [1,2-Dimethyl-benzene]	C8.H10	95-47-6	16	2	7	7
39		C3 Alkyl benzene [1,2,4-Trimethyl-benzene]	C9.H12	95-63-6	2	0	1	1
40		C3 Alkyl benzene [1-Methylethyl-benzene]	C9.H12	98-82-8	1	0	1	0
41		Propyl-benzene	C9.H12	103-65-1	8	0	5	3
42		C3 Alkyl benzene [1-Methyl-2-ethyl benzene]	C9.H12	611-14-3	3	0	2	1
43		Isomer of tetramethyl benzene [1,2,3,4-Tetramethyl-benzene]	C10.H14	488-23-3	1	0	1	0
44		1-Methyl-3-(1-methylethyl-) benzene	C10.H14	535-77-3	2	0	1	1
45		Naphthalene	C10.H8	91-20-3	1	0	1	0
46		1-Ethylpropyl-benzene	C11.H16	1196-58-3	1	0	1	0
47	Aliphatic Alcohol	3-Methyl-1-butanol	C5.H12.O	123-51-3	29	7	12	10
48		1-Hexanol	C6.H14.O	111-27-3	1	0	1	0
49		Isomer of ethyl hexanol [3-Methyl-1-hexanol]	C7.H16.O	13231-81-7	3	1	1	1
50		2-Ethyl-1-Hexanol	C8.H18.O	104-76-7	7	1	4	2
51		Isomer of octanol [1-Octanol]	C8.H18.O	111-87-5	12	4	4	4
52		Isomer of octanol [1-Octanol]	C8.H18.O	111-87-5	29	9	11	9
53		Unidentified C13.H28.O [1-Tridecanol]	C13.H28.O	112-70-9	1	0	0	1
54	Unsaturated Alcohol	Isomer of Octen-ol [3-Octen-2-ol]	C8.H16.O	57648-55-2	2	0	1	1
55		Isomer of Octen-ol [3-Octen-2-ol]	C8.H16.O	57648-55-2	15	3	5	7
56	Aliphatic Aldehyde	Unidentified C5.H10.O [Pentanal]	C5.H10.O	110-62-3	46	12	17	17
57		Unidentifed C6.H12.O [Hexanal]	C6.H12.O	66-25-1	45	12	17	16
58		C7 Aldehyde [Heptanal]	C7.H14.O	111-71-7	46	12	17	17
59		Nonanal	C9.H18.O	124-19-6	46	12	17	17
60		Decanal	C10.H20.O	112-31-2	43	11	17	15
61	Unsaturated Aldehyde	2-Methyl-propenal	C4.H6.O	78-85-3	1	1	0	0
62		Isomer of Hexenal [2-Hexenal]	C6.H10.O	6728-26-3	21	5	7	9
63		Isomer of Hexenal [2-Hexenal]	C6.H10.O	6728-26-3	32	10	12	10
64		C7 Unsat. aldehyde [2-Heptenal]	C7.H12.O	18829-55-5	46	12	17	17

Table 1 (concluded)

ndex	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS No. (c)	In All Samples	In Each Age Group 0-14	15-44	45+
65		C7 Unsat. aldehyde [2-Heptenal]	C7.H12.O	57266-86-1	23	8	6	9
66		2,4-Heptadienal	C7.H10.O	4313-03-5	32	6	11	15
67		2,4-Nonadienal	C9.H14.O	6750-03-4	29	10	11	8
68		Isomer of decenal [2-Decenal]	C10.H18.O	3913-81-3	1	1	0	0
69		Isomer of decenal [2-Decenal]	C10.H18.O	3913-81-3	25	5	10	10
70		Unsat. aldehyde [2-Decenal]	C10.H18.O	3913-81-3	28	9	11	8
71		Unsat. aldehyde [2-Decenal]	C10.H18.O	3913-81-3	29	9	12	8
72		Unsat. aldehyde [2-Decenal]	C10.H18.O	3913-81-3	45	12	17	16
73		Diene aldehyde [2,4-Decadienal]	C10.H16.O	25152-84-5	1	1	0	0
74		Diene aldehyde [2,4-Decadienal]	C10.H16.O	25152-84-5	15	6	4	5
75		Diene aldehyde [2,4-Dodecadienal]	C12.H20.O	21662-16-8	26	6	10	10
76	Aliphatic Ketone	C7 Ketone [2-Heptanone]	C7.H14.O	110-43-0	36	9	13	14
77		4-Heptanone	C7.H14.O	123-19-3	35	10	12	13
78		Unidentified C7.H12.O [2,2,3-Trimethyl-cyclobutanone]	C7.H12.O	1449-49-6	7	1	5	1
79		C8 Ketone [3-Octanone]	C8.H16.O	106-68-3	1	0	0	1
80		Sat. ketone [2-Decanone]	C10.H20.O	693-54-9	1	1	0	0
81	Unsaturated Ketone	Isomer of Octen-one [3-Octen-2-one]	C8.H14.O	1669-44-9	9	0	5	4
82		C8 Ketone [3-Octen-1-one]	C8.H14.O	1669-44-9	37	11	13	13
83		3,5-Octadien-2-one	C8.H12.O	30086-02-3	8	3	3	2
84		C9 Unsat. ketone [3-Nonen-2-one]	C9.H16.O	14309-57-0	25	10	6	9
85	Aliphatic Ether	Dimethoxy methane	C3.H8.O2	109-87-5	1	0	0	1
86	Aliphatic Ester	Propanoic acid, ethyl ester	C5.H10.O2	105-37-3	29	4	12	13
87		C5 Methyl ester [Butanoic acid, methyl ester]	C5.H10.O2	623-42-7	3	1	0	2
88		Propanoic acid, propyl ester	C6.H12.O2	106-36-5	7	0	3	4
89		Pentanoic acid, methyl ester	C6.H12.O2	624-24-8	1	0	0	1
90		C7 Methyl ester [Hexanoic acid, methyl ester]	C7.H14.O2	106-70-7	42	11	17	14
91		3-Methyl butanoic acid, ethyl ester	C7.H14.O2	108-64-5	16	4	5	7
92		Propanoic acid, butyl ester	C7.H14.O2	590-01-2	2	0	0	2
93		2-Methyl propanoic acid, 1-methylethyl ester	C7.H14.O2	617-50-5	4	0	3	1
94		Acetic acid, pentyl ester	C7.H14.O2	628-63-7	3	1	1	1
95		2-Methyl butanoic acid, ethyl ester	C7.H14.O2	7452-79-1	5	0	2	3
96		C8 Ethyl ester [Hexanoic acid, ethyl ester]	C8.H16.O2	123-66-0	12	4	2	6
97		Acetic acid, hexyl ester	C8.H16.O2	142-92-7	16	5	5	6
98		C8 Ester [3-Methyl butanoic acid, propyl ester]	C8.H16.O2	557-00-6	7	1	3	3
99		C8 Ester [Butanoic acid, 1-Methylpropyl ester]	C8.H16.O2	819-97-6	1	0	1	0
100		C8 Ester [Butanoic acid, 1-Methylpropyl ester]	C8.H16.O2	819-97-6	4	0	3	1
101		Octanoic acid, methyl ester	C9.H18.O2	111-11-5	27	11	9	7
102		Hexanoic acid, 1-methylethyl ester	C9.H18.O2	2311-46-8	1	0	1	0
103		Butanoic acid, pentyl ester	C9.H18.O2	540-18-1	17	6	9	2
104		Hexanoic acid, 2-methylpropyl ester	C10.H20.O2	105-79-3	1	0	0	1
105		Octanoic acid, ethyl ester	C10.H20.O2	106-32-1	36	10	14	12
106		C10 Ester [2-Methyl-propanoic acid, hexyl ester]	C10.H20.O2	2349-07-7	12	3	3	6
107		C11 Ester [Hexanoic acid, pentyl ester]	C11.H22.O2	540-07-8	24	8	9	7
108		C11 Ester [4-Methyl pentanoic acid, pentyl ester]	C11.H22.O2	25415-71-8	6	1	2	3
109		C11 Ester [Hexanoic acid, 2-Methylbutyl ester]	C11.H22.O2	2601-13-0	4	1	3	0
110		Isomer of octanoic acid [3-Methyl-butyl ester]	C13.H26.O2	2035-99-6	24	7	9	8
111	Unsaturated Ester	3-Octen-1-ol, acetate	C10.H18.O2	69668-83-3	1	1	0	0
112	Halocarbon	C5 Bromoalkane [1-Bromopentane]	C5.H11.BR	110-53-2	3	2	0	1
113		3-Bromo-Pentane	C5.H11.BR	1809-10-5	3	1	1	1
114		Brominated alkane ≥ C7 [1-Bromo-heptane]	C7.H15.BR	629-04-9	2	1	1	0
115		Dichlorobutane [1,4-dichlorobutane]	C4.H8.CL2	110-56-5	2	0	1	1
116		2-Bromo-2-chloro-1,1,trifluoro-ethane	C2.H.CL.BR.F3	151-67-7	16	3	7	6
117	Phenol	Isomer of ethyl-phenol [4-Ethyl-phenol]	C8.H10.O	123-07-9	6	4	0	2
118	Heterocycle	Unidentified C9.H14.O [2-Pentyl-furan]	C9.H14.O	3777-69-3	29	11	9	9
119	Sulfide	Dimethyl disulfide	C2.H6.S2	624-92-0	27	4	12	11
120		Dimethyl trisulfide	C2.H6.S3	3658-80-8	2	0	0	2
121	Organo-Silicon	Decamethyl-cyclopentasiloxane	C10.H30.O5.SI5	541-02-6	28	4	11	13

(a) Tentative compound identification is based on search vs. the NBS mass spectral library. Confirmation has not been achieved by comparing retention with an authentic standard. In cases where more than one reference compound successfully matched the unknown spectrum, a general descriptive name is reported and the best ranked NBS name is provided in brackets.

(b) In cases where both a general name and an NBS name is reported, the formula corresponds to the NBS name and may not be applicable to the general name.

(c) In cases where both a general name and an NBS name is reported, the CAS no. corresponds to the NBS name.

Table 2. Compounds Tentatively Identified in the 6% Florisil Semivolatile Organic Analysis Data Set vs. Frequency/Age Group

Index	Compound Class	Compound (a)	Formula (b)	AS Number (c)	In All Samples	In each Age Group 0-14	15-44	45+	In Blanks
I.S.	Internal Standard	D10-Anthracene			44	12	15	17	3
1	Alkane	2,6,10,14-Tetramethyl-hexadecane	C20.H42	638-36-8	24	6	5	13	0
2		2,6,10,14-Tetramethyl-nonadecane	C23.H48	55124-80-6	8	0	4	4	0
3		Alkane ≥ C18 [2,6,10,14,19-Pentamethyl eicosane]	C25.H52	52268-60-5	4	0	0	4	0
4	Saturated Ketone	1,2,4-Cyclopentatrione	C5.H4.O3	15849-14-6	1	1	0	0	0
5	Saturated Ester	12-Methyl-tridecanoic acid, methyl ester	C15.H30.O2	5129-58-8	4	2	1	1	0
6		Nonanedioic acid, bis(1-methylpropyl) ester	C17.H32.O4	57983-36-5	1	0	0	1	0
7		9-Octadecenoic acid, ethyl ester	C20.H38.O2	111-62-6	29	9	9	11	0
8	Sulfide	Methyl 2-methyl-1-(methylthio)butyl disulfide	C7.H16.S3	69078-83-7	6	1	0	5	0
9		Dimethyl trisulfide	C2.H6.S3	3658-80-8	1	0	0	1	0
10	Dipeptide	Glycine, anhydride	C4.H8.O3.N2	4202-74-8	3	3	0	0	0
11	Alkene	C5 Substituted naphthalene [Octahydro-tetramethyl-1H-cyclopropan[A]naphthalene]	C15.H24	17334-55-3	6	1	0	5	0
12		Hexahydro-4,7-dimethyl-1-(1-methylethyl)-naphthalene...	C15.H24	483-76-1	1	0	0	1	0
13		5-Ethylidene-1-methyl-cycloheptene	C10.H16	15402-94-5	34	8	10	16	0
14		C30 Unsat. hydrocarbon [Hexamethyl-tetracosahexaene]	C30.H50	111-02-4	1	0	1	0	0
15		Ylangene	C15.H24	14912-44-8	2	0	0	2	0
16	Unsaturated Aldehyde	2-Butyl-2-octenal	C12.H22.O	13019-16-4	4	2	0	2	0
17		Unidentified C9.H8.O [Cyclooctatetraene-1-carboxaldehyde]	C9.H8.O	30844-12-3	1	0	0	1	0
18	Unsaturated Amine	N,N-Dimethyl-3-octen-2-amine	C10.H21.N	55956-31-5	1	0	1	0	0
19	Unsaturated Ketone	6,10-Dimethyl-5,9-undecadien-2-one	C13.H22.O	3796-70-1	1	0	1	0	0
20	Arene	C4 Alkyl benzene [1-Ethyl-2,3-dimethyl benzene]	C10.H14	933-98-2	1	0	0	1	0
21		2-Ethyl-1,3-dimethyl-benzene	C10.H14	2870-04-4	10	2	3	5	0
22		C4 Alkyl benzene [4-Ethyl-1,2-dimethyl-benzene]	C10.H14	934-80-5	6	0	1	5	0
23		C4 Alkyl benzene [Diethyl benzene]	C10.H14	25340-17-4	6	1	2	3	0
24		C4 Alkyl benzene [Methyl(1-methylethyl)-benzene]	C10.H14	25155-15-1	7	1	2	4	0
25		Cyclohexyl-benzene	C12.H16	827-52-1	3	1	1	1	0
26		C3 Alkyl benzene [1,3,5-Trimethyl-benzene]	C9.H12	108-67-8	3	2	0	1	0
27		C4 Alkyl benzene [1-Ethyl-2,3-dimethyl benzene]	C10.H14	933-98-2	1	0	0	1	0
28		C5 Alkyl benzene [1-Ethyl-4-(1-methylethyl)-benzene]	C11.H16	4218-48-8	1	0	0	1	0
29		C3 Alkyl benzene [1-Ethyl-3-methyl-benzene]	C9.H12	620-14-4	6	1	1	4	0
30		C3 Alkyl benzene [1-Ethyl-2-methyl-benzene]	C9.H12	611-14-3	8	2	0	6	0
31		C3 Alkyl benzene [1,3,5-Trimethyl-benzene	C9.H12	108-67-8	3	1	0	2	0
32		C3 Alkyl benzene [1,3,5-Trimethyl-benzene	C9.H12	108-67-8	5	1	1	3	0
33		C4 Alkyl benzene [1-Ethyl-2,4-dimethyl-benzene]	C10.H14	874-41-9	10	1	2	7	0
34		2-Methyl-naphthalene	C11.H10	91-57-6	1	0	0	1	0
35		Unidentified C10.H12 [2,3-Dihydro-1-methyl-1H-Indene]	C10.H12	767-58-8	1	0	1	0	0
36		Unid. C15.H24 [Hexahydro-tetramethyl-benzocycloheptene]	C15.H24	1461-03-6	1	0	0	1	0
37		Unsat. C4 alkyl benzene [4-Ethenyl-1,2-dimethyl-benzene]	C10.H12	27831-13-6	5	1	1	3	0
38		2-Propenyl-benzene	C9.H10	300-57-2	3	1	0	2	0
39	Aromatic Aldehyde	Benzaldehyde	C7.H6.O	100-52-7	11	11	0	0	0
40		4-Pentyl-benzaldehyde	C12.H16.O	6853-57-2	1	0	1	0	0
41	Aromatic Ketone	Unidentified C9.H8.O [2,3-Dihydro-1H-Inden-1-one]	C9.H8.O	83-33-0	3	0	3	0	0
42		1-Phenyl-ethanone	C8.H8.O	98-86-2	2	0	1	1	0
43	Phenol	2,6-Bis(1,1-dimethylethyl)-4-methyl-phenol	C15.H24.O	128-37-0	8	0	3	5	0
44		[1,1'-Biphenyl]-2-ol	C12.H10.O	90-43-7	2	0	0	2	0
45		2,2'-Methylenebis[6-(1,1-dimethylethyl)-4-methyl-phenol	C23.H32.O2	119-47-1	2	0	0	2	0
46	Aromatic Ester	Benzenepropanoic acid, ethyl ester	C11.H14.O2	2021-28-5	3	0	2	1	0
47	Aromatic Ether	1,1'-Oxybis-benzene	C12.H10.O	101-84-8	33	4	13	16	0
48		1-Methoxy-4-(1-propenyl)-benzene	C10.H12.O	104-46-1	1	1	0	0	0
49	Aromatic Amine	C2 Alkyl benzenamine [3,5-Dimethyl-benzenamine]	C8.H11.N	108-69-0	7	0	0	7	0
50	Aromatic Oxime	4-Methyl benzaldehyde, oxime	C8.H9.O.N	3717-15-5	39	10	13	16	0
51	Thiocyanic Ester	Thiocyanic acid, phenyl ester	C7.H5.N.S	5285-87-0	3	0	1	2	0
52	Heterocyclic Compound	2,3,5-Trimethyl-1H-pyrrole	C7.H11.N	2199-41-9	11	8	0	3	0
53		Unidentified C8.H7.N [1H-Indole]	C8.H7.N	120-72-9	4	0	1	3	0
54		Unidentified C8.H7.N [Indolizine]	C8.H7.N	274-40-8	3	0	1	2	0
55		2-(Methylthio)-benzothiazole	C8.H7.N.S2	615-22-5	1	0	0	1	0
56		5-(2-Propenyl)-1,3-Benzodioxole	C10.H10.O2	94-59-7	1	0	0	1	0
57		1,4-Dioxaspiro[4.6]undec-7-ene	C9.H14.O2	7140-60-5	1	0	0	1	0
58		2,4-Dihydro-2,5-dimethyl-3H-pyrazol-3-one	C5.H8.O.N2	2749-59-9	3	3	0	0	0
59		5,5-Diethyl-2,4-imidazolidinedione	C7.H12.O2.N2	5455-34-5	1	0	0	1	0
60	Steroid	(5.Alpha.)-cholest-3-ene	C27.H46	28338-69-4	9	0	2	7	0
61		(3.Beta.)- Cholest-5-en-3-ol acetate	C29.H48.O2	604-35-3	1	0	1	0	0
62		Cholest-5-en-3-ol- (3.beta.)-, propanoate	C30.H50.O2	633-31-8	1	1	0	0	0
63		Cholest-5-en-3-one	C27.H44.O	601-54-7	3	0	2	1	0
64		Cholest-5-ene	C27.H46	570-74-1	10	2	4	4	0

Table 2 (concluded)

Index	Compound Class	Compound (a)	Formula (b)	AS Number (c)	In All Samples	In each Age Group 0-14	15-44	45+	In Blanks
65		(5.Alpha.)-cholest-7-en-3-one	C27.H44.O	15459-85-5	1	0	1	0	0
66		Cholesta-3,5-dien-7-one	C27.H42.O	567-72-6	1	0	1	0	0
67		(3.Beta.)-cholesta-4,6-dien-3-ol benzoate	C34.H48.O2	25485-34-1	3	0	2	1	0
68		Cholesterol	C27.H46.O	57-88-5	3	0	1	2	0
69		Isomer of cholestenol [5-cholesten-3-ol propionate]	C30.H50.O2	633-31-8	40	9	15	16	0
70		Pregnane, (5.alpha.)-	C21.H36	641-85-	4	1	0	3	0
71		(3.Beta.)-26,27-dinorergost-5-en-3-ol benzoate	C33.H48.O2	58003-48-8	1	0	1	0	0
72	Chlorinated Hydrocarbon	1,1-Dichloro-1-propene	C3.H4.CL2	563-58-6	1	0	1	0	0
73		(4-Chloropnenyl)phenyl-methanone	C13.H9.O.CL	134-85-0	1	0	1	0	0
74		2-Chloro-6-methyl-benzonitrile	C8.H6.N.CL	6575-09-3	1	1	0	0	0
75		Dichlorobenzene [1,3-dichloro-benzene]	C6.H4.Cl2	541-73-1	13	3	1	9	0
76		Lindane	C6.H6.CL6	58-89-9	6	2	0	4	0
77		DDD	C14.H10.CL4	72-54-8	12	4	3	5	0
78	Organo-Silicon	Isomer of decamethyl-cyclopentasiloxane	C10.H30.O5.Si5	541-02-6	28	4	7	17	0
79		Octamethyl-cyclotetrasiloxane	C8.H24.O4.SI4	556-67-2	21	7	3	11	0
80		Isomer of decamethyl-cyclopentasiloxane	C10.H30.O5.SI5	541-02-6	1	0	0	1	0
81	Phthalate	Diheptyl phthalate	C22.H34.O4	3648-21-3	1	0	0	1	0

(a) Tentative compound identification is based on search vs. the NBS mass spectral library. Confirmation has not been achieved by comparing retention with an authentic standard. In cases where more than one reference compound successfully matched the unknown spectrum, a general descriptive name is reported and the best ranked NBS name is provided in brackets.

(b) In cases where both a general name and an NBS name is reported, the formula corresponds to the NBS name and may not be applicable to the general name.

(c) In cases where both a general name and an NBS name is reported, the CAS no. corresponds to the NBS name.

Table 3. Compounds Tentatively Identified in the 15/50% Florisil Semivolatile Organic Analysis Data Set vs. Frequency/Age Group

Index	Compound Class	Compound (a)	Formula (b)	CAS number (c)	Number of Occurrences In All Samples	In each Age Group 0-14	15-44	45+	In Blanks
I.S.	Internal Standard	D10-Anthracene - Internal Standard	C14.D10		46	12	17	17	4
1	Alkane	Unidentified C10.H20 [Diethyl cyclohexane]	C10.H20	1331-43-7	2	0	0	2	3
2	Saturated Ester	1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol, exo propanoate-	C13.H22.O2	2756-56-1	1	0	0	1	0
3		Dodecanoic acid, ethyl ester	C14.H28.O2	106-33-2	4	0	0	4	0
4		Hexanedioic acid,mono(2-ethylhexyl) ester	C14.H26.O4	4337-65-9	1	0	0	1	1
5		Alkyl ester [15-Methyl-heptadecanoate]	C20.H40.O2	57274-46-1	13	1	4	8	0
6	Saturated Polyfunctional	Ethylhydrazone propionaldehyde	C5.H12.N2	7422-92-6	1	1	0	0	0
7		9-Oxo-nonanoic acid, ethyl ester	C11.H20.O3	3433-16-7	2	0	0	2	0
8	Alkene	1-Methyl-3-(1-methylethenyl)-cyclohexene	C10.H16	499-03-6	4	1	2	1	0
9	Unsaturated Aldehyde	Trimethyl-3-cyclohexene-1-carboxaldehyde	C10.H16.O	40702-26-9	3	0	2	1	0
10		2-Butyl-2-octenal	C12.H22.O	13019-16-4	28	10	9	9	0
11	Unsaturated Ketone	3-Methyl-3-Buten-2-one, dimer	C5.H8.O2	54789-11-6	2	2	0	0	0
12		2,4,6-Cycloheptatriene-1-one	C7.H6.O	539-80-0	2	2	0	0	0
13		5-Undecen-4-one	C11.H20.O	56312-55-1	3	1	0	2	0
14		5-Ethyl-2-methyl-4-heptene-3-one	C10.H18.O	49833-96-7	2	1	0	1	0
15	Unsaturated Polyfuntional	Substituted cyclopentenone [Butyl-methoxy-cyclopenten-1-one]	C10.H16.O2	53690-92-9	3	1	0	2	1
16		Substituted cyclopentenone [Butyl-methoxy-cyclopenten-1-one]	C10.H16.O2	53690-92-9	4	1	0	3	1
17		Substituted cyclopentenone [Butyl-methoxy-cyclopenten-1-one]	C10.H16.O2	53690-92-9	23	6	4	13	3
18		2-Methoxy-2-octen-4-one	C9.H16.O2	24985-48-6	2	2	0	0	0
19	Alkyne	5,5-Dimethyl-3-heptyne	C9.H16	23097-98-5	1	1	0	0	0
20	Arene	C3-Alkyl benzene [1,3,5-trimethyl-benzene]	C9.H12	95-63-6	8	4	1	3	0
21		C3 Alkyl benzene [1,2,4-Trimethyl-benzene]	C9.H12	95-63-6	5	3	1	1	0
22		C3-Alkyl benzene [1,2,4-trimethyl-benzene]	C9.H12	108-67-8	1	1	0	0	0
23		C3 Alkyl benzene [1-Ethyl-3-methyl-benzene]	C9.H12	620-14-4	2	0	0	2	0
24		Unidentified C11.H10 [1-Ethylidene-indene]	C11.H10	2471-83-2	2	0	1	1	0
25	Aromatic Aldehyde	Benzaldehyde	C7.H6.O	100-52-7	8	5	1	2	0
26		Unidentified C10.H10.O [.Alpha.-ethylidene-benzeneacetaldehyde]	C10.H10.O	4411-89-6	4	2	1	1	0
27		Unidentified C10.H10.O [.Alpha.-ethylidene-benzeneacetaldehyde]	C10.H10.O	4411-89-6	20	5	7	8	0
28	Aromatic Ketone	1-Phenyl-ethanone	C8.H8.O	98-86-2	4	0	2	2	1
29	Aromatic Amide	N-Methyl-1-naphthalenecarboxamide	C12.H11.O.N	3400-33-7	1	0	0	1	0
30	Aromatic Carboxylate	Benzenepropanoic acid, .beta.,.beta.-dimethyl-	C11.H14.O2	1010-48-6	1	0	1	0	0
31		2-(acetylamino)-benzoic acid,methyl ester	C10.H11.O3.N	2719-60-2	2	1	0	1	0
32		Benzenepropanoic acid, ethyl ester	C11.H14.O2	1010-48-6	5	1	4	0	0
33		Benzenepropanoic acid	C9.H10.O2	501-52-0	1	0	0	1	0
34	Phthalic Acid Derivative	Butyl decyl phthalate	C22.H34.O4	89-19-0	11	3	4	4	4
35		Isomer of diheptyl phthalate	C22.H34.O4	3648-21-3	2	1	1	0	0
36		Isomer of diheptyl phthalate	C22.H34.O4	3648-21-3	3	1	2	0	0
37		Butyl phthalate, ester with butyl glycolate	C18.H24.O6	85-70-1	6	2	1	3	2
38		Unidentified phthalate			3	0	1	2	0
39	Phenol	Methyl phenol [2-Methyl-phenol]	C7.H8.O	95-48-7	5	0	0	5	0
40		[1,1'-Biphenyl]-2-ol	C12.H10.O	90-43-7	18	3	6	9	0
41		2-Naphthalenol	C10.H8.O	135-19-3	1	0	0	1	0
42	Aromatic Polyfunctional	1,3-Dimethoxy-benzene	C8.H10.O2	151-10-0	2	1	0	1	0
43		1-Phenyl-1,2-butanediol	C10.H14.O2	22607-13-2	2	1	0	1	0
44		2-Ethoxy-benzaldenyde	C9.H10.O2	613-69-4	4	2	1	1	0
45		Unidentified C7.H5.O.N.S [Thiocyanic acid, 4-hydroxyphenyl ester	C7.H5.O.N.S	3774-52-5	1	1	0	0	0
46	Drug	Methaqualone	C16.H14.O.N2	72-44-6	4	0	4	0	0
47		Unidentified barbiturate [5-Ethyl-1,3-dimethyl pyrimidinetrione]	C8.H12.O3.N2	7391-61-9	1	0	0	1	0
48		Alkyl substituted pyrimidinetrione [Mephobarbital]	C13.H14.O3.N2	115-38-8	3	2	1	0	0
49		Alkyl substituted pyrimidinetrione [Pentobarbital]	C11.H18.O3.N2	76-74-4	19	5	8	6	0
50		Alkyl substituted pyrimidinetrione [Phenobarbital]	C12.H12.O3.N2	50-06-6	5	3	1	1	0
51		Alkyl substituted pyrimidinetrione [Metharbital]	C9.H14.O3.N2	50-11-3	1	0	0	1	0
52		Alkyl substituted pyrimidinetrione [Metharbital]	C9.H14.O3.N2	50-11-3	3	1	1	1	0
53	Heterocyclic Compound	1,7-Naphthyridine	C8.H6.N2	253-69-0	3	0	2	1	0
54		Isomer of dimethyl-piperidine [1,4-Dimethyl-piperidine]	C7.H15.N	695-15-8	11	9	2	0	0
55		3-Pyridinecarboxaldehyde, oxime	C6.H6.O.N2	51892-16-1	10	5	4	1	1
56		4-Pyridinecarboxaldehyde	C6.H5.O.N	872-85-5	1	1	0	0	0
57		Unidentified C8.H7.N [Indolizine]	C8.H7.N	274-40-8	2	0	0	2	0
58		C2 Alkyl pyrazine [2,6-Dimethyl pyrizine]	C6.H8.N2	108-50-9	3	3	0	0	0
59		2-Methoxy-3-methyl-pyrazine	C6.H8.O.N2	2882-21-5	7	3	1	3	0
60		1,2-Benzisothiazole	C7.H5.N.S	272-16-2	4	0	0	4	0
61		Unidentified C7.H11.N.S [2-Methyl-4-propyl-thiazole]	C7.H11.N.S	41981-63-9	8	0	0	8	1
62		Alkyl thazole [4-Ethyl-5-methyl-thiazole]	C6.H9.N.S	52414-91-2	5	3	0	2	1
63		4-Propyl-thiazole	C6.H9.N.S	41981-60-6	3	2	0	1	0

Table 3 (concluded)

Index	Compound Class	Compound (a)	Formula (b)	CAS number (c)	Number of Occurrences In All Samples	In each Age Group 0-14	15-44	45+	In Blanks
64		1,3-Benzodioxole	C7.H6.O2	274-09-9	2	0	0	2	0
65		4,7-Dimethyl-3(2H)-benzofuranone	C10.H10.O2	20895-45-8	4	1	0	3	0
66		Unid. C11.H16.O2 [Tetrahydro-trimethyl-2(4H)-benzofuranone]	C11.H16.O2	17092-92-1	6	0	2	4	0
67		5-(Butylimino)-2(5H)-furanone	C8.H11.O2.N	27396-39-0	3	0	2	1	0
68		2H-1-Benzopyran-2-one	C9.H6.O2	91-64-5	1	0	0	1	0
69		1,3,5-Trimethyl-1H-pyrazole	C6.H10.N2	1072-91-9	1	0	0	1	1
70		Isomer of thienyl-ethanone [1-(3-Thienyl)-ethanone]	C6.H6.O.S	1468-83-3	7	4	0	3	0
71		1-(4-Hydroxy-3-thienyl)-ethanone	C6.H6.O2.S	5556-16-1	3	2	1	0	0
72		2,3,4-trimethyl thiophene	C7.H10.S	1795-04-6	5	0	2	3	0
73		2-Methyl-5-propyl-thiophene	C8.H12.S	33933-73-2	4	2	2	0	0
74		2-t-Butoxy-thiophene	C8.H12.O.S	23290-55-3	4	3	0	1	0
75	Steroid	Isomer of cholest-en-ol [Cholest-5-en-3-ol,acetate]	C29.H48.O2	604-35-3	37	12	14	11	1
76		Isomer of cholest-en-ol [Cholest-5-en-3-ol,acetate]	C29.H48.O2	604-35-3	25	6	7	12	0
77		Cholest-5-en-3-ol (3.beta.)-, propanoate	C30.H50.O2	604-35-3	45	12	17	16	2
78		Cholest-5-en-3-one	C27.H44.O	601-54-7	44	11	17	16	2
79		Cholest-5-ene	C27.H46	570-74-1	30	5	11	14	0
80		Isomer of cholest-en-ol [4-Methyl-cholest-8(14)-en-3-ol]	C28.H48.O	62014-96-4	5	0	4	1	0
81		Cholesta-3,5-dien-7-one	C27.H42.O	567-72-6	22	8	6	8	1
82		Cholesta-4,6-dien-3-ol (3.Beta.), Benzoate	C34.H48.O2	633-31-8	45	12	17	16	2
83		Cholesta-5,7-dien-3-ol, (3.beta.)	C27.H44.O	434-16-2	3	0	0	3	0
84		Isomer of cholestanol [Cholestanol]	C27.H48.O	80-97-7	23	5	10	8	0
85		Methyl-cholestan-3-ol, (3.beta.,5.alpha.,6.beta.)-	C28.H50.O	43217-65-8	15	3	4	8	0
86		3-(Acetoxy)-cholestan-6-one, (3.beta,5.alpha.)-	C29.H48.O3	1256-83-3	3	1	2	0	0
87		Cholestane-3,5-diol, (3.beta.,5.alpha.)-	C27.H48.O2	3347-60-2	2	1	0	1	0
88		Cholestanol	C27.H48.O	80-97-7	4	0	0	4	0
89		Cholesterol	C27.H46.O	57-88-5	44	12	17	15	1
90	Halogenated Hydrocarbon	1-Chloro-4-(Methylsulfonyl)-benzene	C7.H7.O2.S.CL	98-57-7	1	0	0	1	0
91		Isomer of fluoro-methyl-benzene [1-Fluoro-2-methyl-benzene]	C7.H7.F	95-52-3	10	2	3	5	1
92		Carbonochloridothioic acid, S-methyl ester	C2.H3.O.S.CL	2812-72-8	5	4	1	0	0
93		1,1-Dichloro-ethene	C2.H2.CL2	75-35-4	1	1	0	0	0
94		4-Chloro-2-(phenylmethyl)-phenol	C13.H11.O.CL	120-32-1	4	1	0	3	0
95	Organo-Silicon	1-Butynyl-trimethyl silane	C7.H14.SI	62108-37-6	7	4	2	1	0
96		Trimethyl[(1-methyl-2-propynyl)oxy]-silane	C7.H14.O.SI	17869-76-0	5	2	1	2	0

(a) Tentative compound identification is based on search vs. the NBS mass spectral library. Confirmation has not been achieved by comparing retention with an authentic standard. In cases where more than one reference compound successfully matched the unknown spectrum, a general descriptive name is reported and the best ranked NBS name is provided in brackets.

(b) In cases where both a general name and an NBS name is reported, the formula corresponds to the NBS name and may not be applicable to the general name.

(c) In cases where both a general name and an NBS name is reported, the CAS no. corresponds to the NBS name.

Table 4. Compounds Tentatively Identified in the Volatile Organic Analysis Data Set vs. Frequency/Census Region

Index	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS No. (c)	Total Number of Occurrences	Number of Occurrences in Each Region			
						NC	NE	S	W
I.S.	Internal Standard	Bromochloropropane - Internal Standard			46	12	9	19	6
1	Carbon Dioxide	Carbon dioxide	C.O2	124-38-9	45	11	9	19	6
2	Alkane	2-Methyl-butane	C5.H12	78-78-4	18	4	5	6	3
3		Unidentified C5.H10 [Cyclopentane]	C5.H10	287-92-3	7	1	1	4	1
4		C3 Substituted cyclopropane [Propyl-cyclopropane]	C6.H12	2415-72-7	13	5	1	7	0
5		C3 Substituted cyclopropane [Propyl-cyclopropane]	C6.H12	2415-72-7	22	6	5	11	0
6		2,3-Dimethyl-hexane	C8.H18	584-94-1	31	8	7	13	3
7		1,2-Diethyl-cyclobutane	C8.H16	61141-83-1	3	0	0	3	0
8		Alkane ≥ C10 [Decane]	C10.H22	124-18-5	16	7	2	7	0
9		C10 Alkane [2-Methyl-nonane]	C10.H22	871-83-0	9	4	3	0	2
10		2,2,3,3-Tetramethyl-hexane	C10.H22	13475-81-5	10	2	4	3	1
11		Sat. alkane ≥ C11 [2-Methyl-decane]	C11.H24	6975-98-0	6	2	0	4	0
12		Alkyl substituted hexane [Pentyl-cyclohexane]	C11.H22	4292-92-6	1	0	0	0	1
13		2,2-Dimethyl-decane	C12.H26	17302-37-3	13	6	1	5	1
14		C13 Alkane [3,3-Dimethyl-undecane]	C13.H28	17312-65-1	1	1	0	0	0
15		Alkane [6-Ethyl-2-methyl-decane]	C13.H28	62108-21-8	8	1	3	2	2
16		Alkane [2,6,7-Trimethyl-decane]	C13.H28	62108-25-2	21	4	3	13	1
17		Alkane ≥ C11 [5-(1-Methylpropyl)-nonane]	C13.H28	62185-54-0	1	1	0	0	0
18		C13 Alkane [2,2,7-Trimethyl-decane]	C13.H28	62237-99-4	10	4	0	6	0
19		3,3,8-Trimethyl-decane	C13.H28	62338-16-3	1	1	0	0	0
20		Alkane [6-Methyl-tridecane]	C14.H30	13287-21-3	4	3	0	1	0
21	Alkene	C5 Alkane [1-Pentene]	C5.H10	109-67-1	4	0	0	4	0
22		1-Hexene	C6.H12	592-41-6	15	4	2	5	4
23		Unidentified C6.H12 [1-Hexene]	C6.H12	592-41-6	24	7	5	11	1
24		3-Methyl-1,4-heptadiene	C8.H14	1603-01-6	4	2	0	1	1
25		1,6-Octadiene	C8.H14	3710-41-6	4	2	1	0	1
26		1,3,6-Octatriene	C8.H12	22038-69-3	10	4	3	1	2
27		Unidentified C8.H12 [3-Ethylidene-1-methyl-cyclopentene]	C8.H12	62338-00-5	1	0	0	0	1
28		1-Nonene	C9.H18	124-11-8	8	2	2	4	0
29		3-Ethyl-2-methyl-1,3-hexadiene	C9.H16	61142-36-7	44	10	9	19	6
30		C10 Ringed alkane [1,7,7-Trimethyl-bicyclo[2.2.1]hept-2-ene]	C10.H16	464-17-5	44	11	8	19	6
31		1-Methyl-4-(1-methylethenyl)-cyclohexene	C10.H16	5989-54-8	1	1	0	0	0
32		7-(1-Methylethylidene)-bicyclo[4.1.0] heptane	C10.H16	53282-47-6	1	0	0	0	1
33		C11 Alkene [1-Undecene]	C11.H22	821-95-4	8	1	0	4	3
34		C11 Alkene [1-Ethenyl-2-hexenyl-cyclopropane]	C11.H8	22822-99-7	2	0	0	1	1
35		Isomer of Undecen-3-yne [5-Undec-3-yne]	C11.H18	74744-31-3	17	6	2	6	3
36		Isomer of Undecen-3-yne [5-Undec-3-yne]	C11.H18	74744-31-3	31	8	7	12	4
37	Arene	C2 Alkyl benzene [1,2-Dimethyl-benzene]	C8.H10	95-47-6	41	12	9	17	3
38		C2 Alkyl benzene [1,2-Dimethyl-benzene]	C8.H10	95-47-6	16	8	1	7	0
39		C3 Alkyl benzene [1,2,4-Trimethyl-benzene]	C9.H12	95-63-6	2	0	0	2	0
40		C3 Alkyl benzene [1-Methylethyl-benzene]	C9.H12	98-82-8	1	1	0	0	0
41		Propyl-benzene	C9.H12	103-65-1	8	2	0	6	0
42		C3 Alkyl benzene [1-Methyl-2-ethyl benzene]	C9.H12	611-14-3	3	1	0	2	0
43		Isomer of tetramethyl benzene [1,2,3,4-Tetramethyl-benzene]	C10.H14	488-23-3	1	0	0	1	0
44		1-Methyl-3-(1-methylethyl-) benzene	C10.H14	535-77-3	2	2	0	0	0
45		Naphthalene	C10.H8	91-20-3	1	0	0	1	0
46		1-Ethylpropyl-benzene	C11.H16	1196-58-3	1	1	0	0	0
47	Aliphatic Alcohol	3-Methyl-1-butanol	C5.H12.O	123-51-3	29	11	5	10	3
48		1-Hexanol	C6.H14.O	111-27-3	1	1	0	0	0
49		Isomer of ethyl hexanol [3-Methyl-1-hexanol]	C7.H16.O	13231-81-7	3	0	1	1	1
50		2-Ethyl-1-Hexanol	C8.H18.O	104-76-7	7	3	1	2	1
51		Isomer of octanol [1-Octanol]	C8.H18.O	111-87-5	12	3	1	7	1
52		Isomer of octanol [1-Octanol]	C8.H18.O	111-87-5	29	6	8	10	5
53		Unidentified C13.H28.O [1-Tridecanol]	C13.H28.O	112-70-9	1	1	0	0	0
54	Unsaturated Alcohol	Isomer of Octen-ol [3-Octen-2-ol]	C8.H16.O	57648-55-2	2	0	0	2	0
55		Isomer of Octen-ol [3-Octen-2-ol]	C8.H16.O	57648-55-2	15	7	2	5	1
56	Aliphatic Aldehyde	Unidentified C5.H10.O [Pentanal]	C5.H10.O	110-62-3	46	12	9	19	6
57		Unidentifed C6.H12.O [Hexanal]	C6.H12.O	66-25-1	45	12	9	18	6
58		C7 Aldehyde [Heptanal]	C7.H14.O	111-71-7	46	12	9	19	6
59		Nonanal	C9.H18.O	124-19-6	46	12	9	19	6
60		Decanal	C10.H20.O	112-31-2	43	11	9	18	5
61	Unsaturated Aldehyde	2-Methyl-propenal	C4.H6.O	78-85-3	1	0	0	1	0
62		Isomer of Hexenal [2-Hexenal]	C6.H10.O	6728-26-3	21	3	5	10	3
63		Isomer of Hexenal [2-Hexenal]	C6.H10.O	6728-26-3	32	6	9	13	4
64		C7 Unsat. aldehyde [2-Heptenal]	C7.H12.O	18829-55-5	46	12	9	19	6
65		C7 Unsat. aldehyde [2-Heptenal]	C7.H12.O	57266-86-1	23	7	4	8	4
66		2,4-Heptadienal	C7.H10.O	4313-03-5	32	9	8	12	3
67		2,4-Nonadienal	C9.H14.O	6750-03-4	29	7	9	10	3

Table 4 (concluded)

Index	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS No. (c)	Total Number of Occurrences	Number of Occurrences in Each Region NC	NE	S	W
68		Isomer of decenal [2-Decenal]	C10.H18.O	3913-81-3	1	0	0	1	0
69		Isomer of decenal [2-Decenal]	C10.H18.O	3913-81-3	25	8	6	7	4
70		Unsat. aldehyde [2-Decenal]	C10.H18.O	3913-81-3	28	4	4	14	6
71		Unsat. aldehyde [2-Decenal]	C10.H18.O	3913-81-3	29	6	7	12	4
72		Unsat. aldehyde [2-Decenal]	C10.H18.O	3913-81-3	45	12	9	18	6
73		Diene aldehyde [2,4-Decadienal]	C10.H16.O	25152-84-5	1	0	0	0	1
74		Diene aldehyde [2,4-Decadienal]	C10.H16.O	25152-84-5	15	1	4	6	4
75		Diene aldehyde [2,4-Dodecadienal]	C12.H20.O	21662-16-8	26	8	5	11	2
76	Aliphatic Ketone	C7 Ketone [2-Heptanone]	C7.H14.O	110-43-0	36	10	6	15	5
77		4-Heptanone	C7.H14.O	123-19-3	35	12	8	11	4
78		Unidentified C7.H12.O [2,2,3-Trimethyl-cyclobutanone]	C7.H12.O	1449-49-6	7	2	2	2	1
79		C8 Ketone [3-Octanone]	C8.H16.O	106-68-3	1	1	0	0	0
80		Sat. ketone [2-Decanone]	C10.H20.O	693-54-9	1	1	0	0	0
81	Unsaturated Ketone	Isomer of Octen-one [3-Octen-2-one]	C8.H14.O	1669-44-9	9	1	2	6	0
82		C8 Ketone [3-Octen-1-one]	C8.H14.O	1669-44-9	37	11	8	13	5
83		3,5-Octadien-2-one	C8.H12.O	30086-02-3	8	2	0	6	0
84		C9 Unsat. ketone [3-Nonen-2-one]	C9.H16.O	14309-57-0	25	5	7	9	4
85	Aliphatic Ether	Dimethoxy methane	C3.H8.O2	109-87-5	1	0	1	0	0
86	Aliphatic Ester	Propanoic acid, ethyl ester	C5.H10.O2	105-37-3	29	11	4	12	2
87		C5 Methyl ester [Butanoic acid, methyl ester]	C5.H10.O2	623-42-7	3	1	0	1	1
88		Propanoic acid, propyl ester	C6.H12.O2	106-36-5	7	4	0	2	1
89		Pentanoic acid, methyl ester	C6.H12.O2	624-24-8	1	1	0	0	0
90		C7 Methyl ester [Hexanoic acid, methyl ester]	C7.H14.O2	106-70-7	42	10	8	18	6
91		3-Methyl butanoic acid, ethyl ester	C7.H14.O2	108-64-5	16	10	0	5	1
92		Propanoic acid, butyl ester	C7.H14.O2	590-01-2	2	1	0	1	0
93		2-Methyl propanoic acid, 1-methylethyl ester	C7.H14.O2	617-50-5	4	2	0	2	0
94		Acetic acid, pentyl ester	C7.H14.O2	628-63-7	3	1	1	1	0
95		2-Methyl butanoic acid, ethyl ester	C7.H14.O2	7452-79-1	5	2	0	3	0
96		C8 Ethyl ester [Hexanoic acid, ethyl ester]	C8.H16.O2	123-66-0	12	3	3	4	2
97		Acetic acid, hexyl ester	C8.H16.O2	142-92-7	16	4	1	9	2
98		C8 Ester [3-Methyl butanoic acid, propyl ester]	C8.H16.O2	557-00-6	7	4	0	3	0
99		C8 Ester [Butanoic acid, 1-Methylpropyl ester]	C8.H16.O2	819-97-6	1	1	0	0	0
100		C8 Ester [Butanoic acid, 1-Methylpropyl ester]	C8.H16.O2	819-97-6	4	2	0	2	0
101		Octanoic acid, methyl ester	C9.H18.O2	111-11-5	27	7	8	8	4
102		Hexanoic acid, 1-methylethyl ester	C9.H18.O2	2311-46-8	1	0	0	1	0
103		Butanoic acid, pentyl ester	C9.H18.O2	540-18-1	17	4	3	7	3
104		Hexanoic acid, 2-methylpropyl ester	C10.H20.O2	105-79-3	1	0	0	1	0
105		Octanoic acid, ethyl ester	C10.H20.O2	106-32-1	36	12	8	11	5
106		C10 Ester [2-Methyl-propanoic acid, hexyl ester]	C10.H20.O2	2349-07-7	12	5	2	4	1
107		C11 Ester [Hexanoic acid, pentyl ester]	C11.H22.O2	540-07-8	24	5	7	10	2
108		C11 Ester [4-Methyl pentanoic acid, pentyl ester]	C11.H22.O2	25415-71-8	6	3	0	2	1
109		C11 Ester [Hexanoic acid, 2-Methylbutyl ester]	C11.H22.O2	2601-13-0	4	3	0	1	0
110		Isomer of octanoic acid [3-Methyl-butyl ester]	C13.H26.O2	2035-99-6	24	6	4	9	5
111	Unsaturated Ester	3-Octen-1-ol, acetate	C10.H18.O2	69668-83-3	1	1	0	0	0
112	Halocarbon	C5 Bromoalkane [1-Bromopentane]	C5.H11.BR	110-53-2	3	1	0	1	1
113		3-Bromo-Pentane	C5.H11.BR	1809-10-5	3	1	0	0	2
114		Brominated alkane ≥ C7 [1-Bromo-heptane]	C7.H15.BR	629-04-9	2	1	0	1	0
115		Dichlorobutane [1,4-dichlorobutane]	C4.H8.CL2	110-56-5	2	1	0	1	0
116		2-Bromo-2-chloro-1,1,trifluoro-ethane	C2.H.CL.BR.F3	151-67-7	16	7	1	5	3
117	Phenol	Isomer of ethyl-phenol [4-Ethyl-phenol]	C8.H10.O	123-07-9	6	1	1	3	1
118	Heterocycle	Unidentified C9.H14.O [2-Pentyl-furan]	C9.H14.O	3777-69-3	29	8	8	9	4
119	Sulfide	Dimethyl disulfide	C2.H6.S2	624-92-0	27	11	1	13	2
120		Dimethyl trisulfide	C2.H6.S3	3658-80-8	2	2	0	0	0
121	Organo-Silicon	Decamethyl-cyclopentasiloxane	C10.H30.O5.SI5	541-02-6	28	7	2	14	5

(a) Tentative compound identification is based on search vs. the NBS mass spectral library. Confirmation has not been achieved by comparing retention with an authentic standard. In cases where more than one reference compound successfully matched the unknown spectrum, a general descriptive name is reported and the best ranked NBS name is provided in brackets.

(b) In cases where both a general name and an NBS name is reported, the formula corresponds to the NBS name and may not be applicable to the general name.

(c) In cases where both a general name and an NBS name is reported, the CAS no. corresponds to the NBS name.

Table 5. Compounds Tentatively Identified in the 6% Florisil Semivolatile Organic Analysis Data Set vs. Frequency/Census Region

Index	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS Number (c)	Total Number of Occurrences		Number of Occurrences in Each Region			
					Samples	Blanks	NC	NE	S	W
I.S	Internal Standard	D10-Anthracene			44	3	12	9	18	5
1	Alkane	2,6,10,14-Tetramethyl-hexadecane	C20.H42	638-36-8	24	0	9	2	12	1
2		2,6,10,14-Tetramethyl-nonadecane	C23.H48	55124-80-6	8	0	3	2	3	0
3		Alkane ≥ C18 [2,6,10,14,19-Pentamethyl eicosane]	C25.H52	52268-60-5	4	0	1	1	2	0
4	Saturated Ketone	1,2,4-Cyclopentatrione	C5.H4.O3	15849-14-6	1	0	0	0	0	1
5	Saturated Ester	12-Methyl-tridecanoic acid, methyl ester	C15.H30.O2	5129-58-8	4	0	1	1	1	1
6		Nonanedioic acid, bis(1-methylpropyl) ester	C17.H32.O4	57983-36-5	1	0	0	0	0	1
7		9-Octadecenoic acid, ethyl ester	C20.H38.O2	111-62-6	29	0	11	3	12	3
8	Sulfide	Methyl 2-methyl-1-(methylthio)butyl disulfide	C7.H16.S3	69078-83-7	6	0	3	1	2	0
9		Dimethyl trisulfide	C2.H6.S3	3658-80-8	1	0	1	0	0	0
10	Dipeptide	Glycine, anhydride	C4.H8.O3.N2	4202-74-8	3	0	1	0	0	2
11	Alkene	C5 Substituted naphthalene [Octahydro-tetramethyl-1H-cyclopropan[A]naphthalene]	C15.H24	17334-55-3	6	0	1	1	2	2
12		Hexahydro-4,7-dimethyl-1-(1-methylethyl)-naphthalene...	C15.H24	483-76-1	1	0	0	1	0	0
13		5-Ethylidene-1-methyl-cycloheptene	C10.H16	15402-94-5	34	0	9	7	13	5
14		C30 Unsat. hydrocarbon [Hexamethyl-tetracosahexaene]	C30.H50	111-02-4	1	0	1	0	0	0
15		Ylangene	C15.H24	14912-44-8	2	0	0	1	0	1
16	Unsaturated Aldehyde	2-Butyl-2-octenal	C12.H22.O	13019-16-4	4	0	0	3	1	0
17		Unidentified C9.H8.O [Cyclooctatetraene-1-carboxaldehyde]	C9.H8.O	30844-12-3	1	0	0	1	0	0
18	Unsaturated Amine	N,N-Dimethyl-3-octen-2-amine	C10.H21.N	55956-31-5	1	0	0	0	0	1
19	Unsaturated Ketone	6,10-Dimethyl-5,9-undecadien-2-one	C13.H22.O	3796-70-1	1	0	0	0	0	1
20	Arene	C4 Alkyl benzene [1-Ethyl-2,3-dimethyl benzene]	C10.H14	933-98-2	1	0	0	0	1	0
21		2-Ethyl-1,3-dimethyl-benzene	C10.H14	2870-04-4	10	0	2	0	8	0
22		C4 Alkyl benzene [4-Ethyl-1,2-dimethyl-benzene]	C10.H14	934-80-5	6	0	1	0	5	0
23		C4 Alkyl benzene [Diethyl benzene]	C10.H14	25340-17-4	6	0	1	0	5	0
24		C4 Alkyl benzene [Methyl(1-methylethyl)-benzene]	C10.H14	25155-15-1	7	0	1	0	6	0
25		Cyclohexyl-benzene	C12.H16	827-52-1	3	0	0	0	0	3
26		C3 Alkyl benzene [1,3,5-Trimethyl-benzene]	C9.H12	108-67-8	3	0	0	0	2	1
27		C4 Alkyl benzene [1-Ethyl-2,3-dimethyl benzene]	C10.H14	933-98-2	1	0	0	0	1	0
28		C5 Alkyl benzene [1-Ethyl-4-(1-methylethyl)-benzene]	C11.H16	4218-48-8	1	0	0	0	1	0
29		C3 Alkyl benzene [1-Ethyl-3-methyl-benzene]	C9.H12	620-14-4	6	0	1	0	5	0
30		C3 Alkyl benzene [1-Ethyl-2-methyl-benzene]	C9.H12	611-14-3	8	0	2	1	5	0
31		C3 Alkyl benzene [1,3,5-Trimethyl-benzene	C9.H12	108-67-8	3	0	1	0	2	0
32		C3 Alkyl benzene [1,3,5-Trimethyl-benzene	C9.H12	108-67-8	5	0	0	0	4	1
33		C4 Alkyl benzene [1-Ethyl-2,4-dimethyl-benzene]	C10.H14	874-41-9	10	0	2	1	7	0
34		2-Methyl-naphthalene	C11.H10	91-57-6	1	0	0	0	1	0
35		Unidentified C10.H12 [2,3-Dihydro-1-methyl-1H-Indene]	C10.H12	767-58-8	1	0	0	0	1	0
36		Unidentified C15.H24 [Hexahydro-tetramethyl-1H-benzocycloheptene]	C15.H24	1461-03-6	1	0	0	0	1	0
37		Unsat. C4 alkyl benzene [4-Ethenyl-1,2-dimethyl-benzene]	C10.H12	27831-13-6	5	0	0	0	5	0
38		2-Propenyl-benzene	C9.H10	300-57-2	3	0	0	0	3	0
39	Aromatic Aldehyde	Benzaldehyde	C7.H6.O	100-52-7	11	0	2	3	4	2
40		4-Pentyl-benzaldehyde	C12.H16.O	6853-57-2	1	0	0	0	0	1
41	Aromatic Ketone	Unidentified C9.H8.O [2,3-Dihydro-1H-Inden-1-one]	C9.H8.O	83-33-0	3	0	1	1	0	1
42		1-Phenyl-ethanone	C8.H8.O	98-86-2	2	0	0	1	0	1
43	Phenol	2,6-Bis(1,1-dimethylethyl)-4-methyl-phenol	C15.H24.O	128-37-0	8	0	1	1	6	0
44		[1,1'-Biphenyl]-2-ol	C12.H10.O	90-43-7	2	0	0	1	0	1
45		2,2'-Methylenebis[6-(1,1-dimethylethyl)-4-methyl-phenol	C23.H32.O2	119-47-1	2	0	0	0	0	2
46	Aromatic Ester	Benzenepropanoic acid, ethyl ester	C11.H14.O2	2021-28-5	3	0	1	0	2	0
47	Aromatic Ether	1,1'-Oxybis-benzene	C12.H10.O	101-84-8	33	0	8	6	16	3
48		1-Methoxy-4-(1-propenyl)-benzene	C10.H12.O	104-46-1	1	0	1	0	0	0
49	Aromatic Amine	C2 Alkyl benzenamine [3,5-Dimethyl-benzenamine]	C8.H11.N	108-69-0	7	0	4	0	1	2
50	Aromatic Oxime	4-Methyl benzaldehyde, oxime	C8.H9.O.N	3717-15-5	39	0	12	7	16	4
51	Thiocyanic Ester	Thiocyanic acid, phenyl ester	C7.H5.N.S	5285-87-0	3	0	1	1	1	0
52	Heterocyclic Compound	2,3,5-Trimethyl-1H-pyrrole	C7.H11.N	2199-41-9	11	0	2	3	4	2
53		Unidentified C8.H7.N [1H-Indole]	C8.H7.N	120-72-9	4	0	0	0	4	0
54		Unidentified C8.H7.N [Indolizine]	C8.H7.N	274-40-8	3	0	0	0	2	1
55		2-(Methylthio)-benzothiazole	C8.H7.N.S2	615-22-5	1	0	0	1	0	0
56		5-(2-Propenyl)-1,3-Benzodioxole	C10.H10.O2	94-59-7	1	0	0	1	0	0
57		1,4-Dioxaspiro[4.6]undec-7-ene	C9.H14.O2	7140-60-5	1	0	0	1	0	0
58		2,4-Dihydro-2,5-dimethyl-3H-pyrazol-3-one	C5.H8.O.N2	2749-59-9	3	0	1	0	0	2
59		5,5-Diethyl-2,4-imidazolidinedione	C7.H12.O2.N2	5455-34-5	1	0	0	1	0	0
60	Steroid	(5.Alpha.)-cholest-3-ene	C27.H46	28338-69-4	9	0	2	1	6	0
61		(3.Beta.)- Cholest-5-en-3-ol acetate	C29.H48.O2	604-35-3	1	0	0	0	1	0
62		Cholest-5-en-3-ol- (3.beta.)-, propanoate	C30.H50.O2	633-31-8	1	0	0	1	0	0

Table 5 (concluded)

Index	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS Number (c)	Total Number of Occurrences		Number of Occurrences in Each Region			
					Samples	Blanks	NC	NE	S	W
63		Cholest-5-en-3-one	C27.H44.O	601-54-7	3	0	0	0	2	1
64		Cholest-5-ene	C27.H46	570-74-1	10	0	4	1	4	1
65		(5.Alpha.)-cholest-7-en-3-one	C27.H44.O	15459-85-5	1	0	0	0	1	0
66		Cholesta-3,5-dien-7-one	C27.H42.O	567-72-6	1	0	0	0	1	0
67		(3.Beta.)-cholesta-4,6-dien-3-ol benzoate	C34.H48.O2	25485-34-1	3	0	0	0	2	1
68		Cholesterol	C27.H46.O	57-88-5	3	0	0	1	1	1
69		Isomer of cholesterol [5-cholesten-3-ol propionate]	C30.H50.O2	633-31-8	40	0	12	9	16	3
70		Pregnane, (5.alpha.)-	C21.H36	641-85-	4	0	0	2	1	1
71		(3.Beta.)-26,27-dinorergost-5-en-3-ol benzoate	C33.H48.O2	58003-48-8	1	0	0	0	1	0
72	Chlorinated Hydrocarbons	1,1-Dichloro-1-propene	C3.H4.CL2	563-58-6	1	0	1	0	0	0
73		(4-Chlorophenyl)phenyl-methanone	C13.H9.O.CL	134-85-0	1	0	0	0	0	1
74		2-Chloro-6-methyl-benzonitrile	C8.H6.N.CL	6575-09-3	1	0	1	0	0	0
75		Dichlorobenzene [1,3-dichloro-benzene]	C6.H4.Cl2	541-73-1	13	0	4	2	6	1
76		Lindane	C6.H6.CL6	58-89-9	6	0	2	3	1	0
77		DDD	C14.H10.CL4	72-54-8	12	0	3	1	8	0
78	Organo-Silicon	Isomer of decamethyl-cyclopentasiloxane	C10.H30.O5.Si5	541-02-6	28	0	7	5	12	4
79		Octamethyl-cyclotetrasiloxane	C8.H24.O4.Si4	556-67-2	21	0	3	5	9	4
80		Isomer of decamethyl-cyclopentasiloxane	C10.H30.O5.Si5	541-02-6	1	0	0	0	0	1
81	Phthalate	Diheptyl phthalate	C22.H34.O4	3648-21-3	1	0	0	0	0	1

(a) Tentative compound identification is based on search vs. the NBS mass spectral library. Confirmation has not been achieved by comparing retention with an authentic standard. In cases where more than one reference compound successfully matched the unknown spectrum, a general descriptive name is reported and the best ranked NBS name is provided in brackets.

(b) In cases where both a general name and an NBS name is reported, the formula corresponds to the NBS name and may not be applicable to the general name.

(c) In cases where both a general name and an NBS name is reported, the CAS no. corresponds to the NBS name.

Table 6. Compounds Tentatively Identified in the 15/50% Florisil Semivolatile Organic Analysis Data Set vs. Frequency/Census Region

Index	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS Number (c)	Total Number of Occurrences Samples	Blanks	Number of Occurrences in Each Region NC	NE	S	W
I.S.	Internal Standard	D10-Anthracene - Internal Standard	C14.D10		46	4	12	9	19	6
1	Alkane	Unidentified C10.H20 [Diethyl cyclohexane]	C10.H20	1331-43-7	2	3	1	0	1	0
2	Saturated Ester	1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol, exo propanoate-	C13.H22.O2	2756-56-1	1	0	0	1	0	0
3		Dodecanoic acid, ethyl ester	C14.H28.O2	106-33-2	4	0	2	1	1	0
4		Hexanedioic acid,mono(2-ethylhexyl) ester	C14.H26.O4	4337-65-9	1	1	0	0	1	0
5		Alkyl ester [15-Methyl-heptadecanoate]	C20.H40.O2	57274-46-1	13	0	5	0	8	0
6	Saturated Polyfunctional	Ethylhydrazone propionaldehyde	C5.H12.N2	7422-92-6	1	0	0	0	1	0
7		9-Oxo-nonanoic acid, ethyl ester	C11.H20.O3	3433-16-7	2	0	1	0	1	0
8	Alkene	1-Methyl-3-(1-methylethenyl)-cyclohexene	C10.H16	499-03-6	4	0	0	0	4	0
9	Unsaturated Aldehyde	Trimethyl-3-cyclohexene-1-carboxaldehyde	C10.H16.O	40702-26-9	3	0	1	0	2	0
10		2-Butyl-2-octenal	C12.H22.O	13019-16-4	28	0	7	6	13	2
11	Unsaturated Ketone	3-Methyl-3-Buten-2-one, dimer	C5.H8.O2	54789-11-6	2	0	1	0	1	0
12		2,4,6-Cycloheptatriene-1-one	C7.H6.O	539-80-0	2	0	0	2	0	0
13		5-Undecen-4-one	C11.H20.O	56312-55-1	3	0	0	3	0	0
14		5-Ethyl-2-methyl-4-heptene-3-one	C10.H18.O	49833-96-7	2	0	0	2	0	0
15	Unsaturated Polyfuntional	Substituted cyclopentenone [Butyl-methoxy-cyclopenten-1-one]	C10.H16.O2	53690-92-9	3	1	2	0	1	0
16		Substituted cyclopentenone [Butyl-methoxy-cyclopenten-1-one]	C10.H16.O2	53690-92-9	4	1	2	1	1	0
17		Substituted cyclopentenone [Butyl-methoxy-cyclopenten-1-one]	C10.H16.O2	53690-92-9	23	3	7	4	7	5
18		2-Methoxy-2-octen-4-one	C9.H16.O2	24985-48-6	2	0	1	0	1	0
19	Alkyne	5,5-Dimethyl-3-heptyne	C9.H16	23097-98-5	1	0	0	0	1	0
20	Arene	C3-Alkyl benzene [1,3,5-trimethyl-benzene]	C9.H12	95-63-6	8	0	2	1	2	3
21		C3 Alkyl benzene [1,2,4-Trimethyl-benzene]	C9.H12	95-63-6	5	0	2	2	1	0
22		C3-Alkyl benzene [1,2,4-trimethyl-benzene]	C9.H12	108-67-8	1	0	0	0	1	0
23		C3 Alkyl benzene [1-Ethyl-3-methyl-benzene]	C9.H12	620-14-4	2	0	0	0	2	0
24		Unidentified C11.H10 [1-Ethylidene-indene]	C11.H10	2471-83-2	2	0	1	1	0	0
25	Aromatic Aldehyde	Benzaldehyde	C7.H6.O	100-52-7	8	0	3	0	3	2
26		Unidentified C10.H10.O [.Alpha.-ethylidene-benzeneacetaldehyde]	C10.H10.O	4411-89-6	4	0	1	1	1	1
27		Unidentified C10.H10.O [.Alpha.-ethylidene-benzeneacetaldehyde]	C10.H10.O	4411-89-6	20	0	6	7	6	1
28	Aromatic Ketone	1-Phenyl-ethanone	C8.H8.O	98-86-2	4	1	0	2	2	0
29	Aromatic Amide	N-Methyl-1-naphthalenecarboxamide	C12.H11.O.N	3400-33-7	1	0	0	0	1	0
30	Aromatic Carboxylate Derivative	Benzenepropanoic acid, .beta.,.beta.-dimethyl-	C11.H14.O2	1010-48-6	1	0	0	0	1	0
31		2-(acetylamino)-benzoic acid,methyl ester	C10.H11.O3.N	2719-60-2	2	0	1	0	1	0
32		Benzenepropanoic acid, ethyl ester	C11.H14.O2	1010-48-6	5	0	2	0	2	1
33		Benzenepropanoic acid	C9.H10.O2	501-52-0	1	0	0	0	1	0
34	Phthalic Acid Derivative	Butyl decyl phthalate	C22.H34.O4	89-19-0	11	4	4	3	4	0
35		Isomer of diheptyl phthalate	C22.H34.O4	3648-21-3	2	0	0	0	2	0
36		Isomer of diheptyl phthalate	C22.H34.O4	3648-21-3	3	0	0	0	3	0
37		Butyl phthalate, ester with butyl glycolate	C18.H24.O6	85-70-1	6	2	3	0	3	0
38		Unidentified phthalate			3	0	0	1	1	1
39	Phenol	Methyl phenol [2-Methyl-phenol]	C7.H8.O	95-48-7	5	0	2	1	1	1
40		[1,1'-Biphenyl]-2-ol	C12.H10.O	90-43-7	18	0	4	6	6	2
41		2-Naphthalenol	C10.H8.O	135-19-3	1	0	0	0	1	0
42	Aromatic Polyfunctional	1,3-Dimethoxy-benzene	C8.H10.O2	151-10-0	2	0	0	1	1	0
43		1-Phenyl-1,2-butanediol	C10.H14.O2	22607-13-2	2	0	0	2	0	0
44		2-Ethoxy-benzaldehyde	C9.H10.O2	613-69-4	4	0	0	2	1	1
45		Unidentified C7.H5.O.N.S [Thiocyanic acid, 4-hydroxyphenyl ester]	C7.H5.O.N.S	3774-52-5	1	0	0	0	0	1
46	Drug	Methaqualone	C16.H14.O.N2	72-44-6	4	0	0	0	4	0
47		Unidentified barbiturate [5-Ethyl-1,3-dimethyl pyrimidinetrione]	C8.H12.O3.N2	7391-61-9	1	0	0	1	0	0
48		Alkyl substituted pyrimidinetrione [Mephobarbital]	C13.H14.O3.N2	115-38-8	3	0	0	1	2	0
49		Alkyl substituted pyrimidinetrione [Pentobarbital]	C11.H18.O3.N2	76-74-4	19	0	6	6	6	1
50		Alkyl substituted pyrimidinetrione [Phenobarbital]	C12.H12.O3.N2	50-06-6	5	0	0	2	3	0
51		Alkyl substituted pyrimidinetrione [Metharbital]	C9.H14.O3.N2	50-11-3	1	0	0	1	0	0
52		Alkyl substituted pyrimidinetrione [Metharbital]	C9.H14.O3.N2	50-11-3	3	0	0	3	0	0
53	Heterocyclic Compound	1,7-Naphthyridine	C8.H6.N2	253-69-0	3	0	2	0	1	0
54		Isomer of dimethyl-piperidine [1,4-Dimethyl-piperidine]	C7.H15.N	695-15-8	11	0	2	2	4	3
55		3-Pyridinecarboxaldehyde, oxime	C6.H6.O.N2	51892-16-1	10	1	4	0	4	2
56		4-Pyridinecarboxaldehyde	C6.H5.O.N	872-85-5	1	0	1	0	0	0
57		Unidentified C8.H7.N [Indolizine]	C8.H7.N	274-40-8	2	0	0	1	1	0
58		C2 Alkyl pyrazine [2,6-Dimethyl pyrizine]	C6.H8.N2	108-50-9	3	0	1	2	0	0
59		2-Methoxy-3-methyl-pyrazine	C6.H8.O.N2	2882-21-5	7	0	2	2	3	0
60		1,2-Benzisothiazole	C7.H5.N.S	272-16-2	4	0	1	1	2	0
61		Unidentified C7.H11.N.S [2-Methyl-4-propyl-thiazole]	C7.H11.N.S	41981-63-9	8	1	3	2	2	1
62		Alkyl thazole [4-Ethyl-5-methyl-thiazole]	C6.H9.N.S	52414-91-2	5	1	1	0	3	1
63		4-Propyl-thiazole	C6.H9.N.S	41981-60-6	3	0	1	1	1	0

Table 6 (concluded)

Index	Compound Class	Compound Name (a)	Compound Formula (b)	Compound CAS Number (c)	Total Number of Occurrences Samples	Blanks	Number of Occurrences in Each Region NC	NE	S	W
64		1,3-Benzodioxole	C7.H6.O2	274-09-9	2	0	1	1	0	0
65		4,7-Dimethyl-3(2H)-benzofuranone	C10.H10.O2	20895-45-8	4	0	2	0	2	0
66		Unidentified C11.H16.O2 [Tetrahydro-trimethyl-2(4H)-benzofuranone]	C11.H16.O2	17092-92-1	6	0	3	0	2	1
67		5-(Butylimino)-2(5H)-furanone	C8.H11.O2.N	27396-39-0	3	0	0	3	0	0
68		2H-1-Benzopyran-2-one	C9.H6.O2	91-64-5	1	0	0	1	0	0
69		1,3,5-Trimethyl-1H-pyrazole	C6.H10.N2	1072-91-9	1	1	0	0	1	0
70		Isomer of thienyl-ethanone [1-(3-Thienyl)-ethanone]	C6.H6.O.S	1468-83-3	7	0	2	2	2	1
71		1-(4-Hydroxy-3-thienyl)-ethanone	C6.H6.O2.S	5556-16-1	3	0	0	0	1	2
72		2,3,4-trimethyl thiophene	C7.H10.S	1795-04-6	5	0	4	0	1	0
73		2-Methyl-5-propyl-thiophene	C8.H12.S	33933-73-2	4	0	1	0	3	0
74		2-t-Butoxy-thiophene	C8.H12.O.S	23290-55-3	4	0	1	0	2	1
75	Steroid	Isomer of cholest-en-ol [Cholest-5-en-3-ol,acetate]	C29.H48.O2	604-35-3	37	1	9	7	16	5
76		Isomer of cholest-en-ol [Cholest-5-en-3-ol,acetate]	C29.H48.O2	604-35-3	25	0	7	8	9	1
77		Cholest-5-en-3-ol (3.beta.)-, propanoate	C30.H50.O2	604-35-3	45	2	12	9	19	5
78		Cholest-5-en-3-one	C27.H44.O	601-54-7	44	2	12	8	19	5
79		Cholest-5-ene	C27.H46	570-74-1	30	0	10	4	14	2
80		Isomer of cholest-en-ol [4-Methyl-cholest-8(14)-en-3-ol]	C28.H48.O	62014-96-4	5	0	3	1	1	0
81		Cholesta-3,5-dien-7-one	C27.H42.O	567-72-6	22	1	5	4	11	2
82		Cholesta-4,6-dien-3-ol (3.Beta.), Benzoate	C34.H48.O2	633-31-8	45	2	12	9	19	5
83		Cholesta-5,7-dien-3-ol, (3.beta.)	C27.H44.O	434-16-2	3	0	2	1	0	0
84		Isomer of cholestanol [Cholestanol]	C27.H48.O	80-97-7	23	0	9	3	11	0
85		Methyl-cholestan-3-ol, (3.beta.,5.alpha.,6.beta.)-	C28.H50.O	43217-65-8	15	0	5	3	6	1
86		3-(Acetoxy)-cholestan-6-one, (3.beta,5.alpha.)-	C29.H48.O3	1256-83-3	3	0	0	0	1	2
87		Cholestane-3,5-diol, (3.beta.,5.alpha.)-	C27.H48.O2	3347-60-2	2	0	1	0	1	0
88		Cholestanol	C27.H48.O	80-97-7	4	0	1	0	2	1
89		Cholesterol	C27.H46.O	57-88-5	44	1	11	9	19	5
90	Halogenated Hydrocarbon	1-Chloro-4-(Methylsulfonyl)-benzene	C7.H7.O2.S.CL	98-57-7	1	0	1	0	0	0
91		Isomer of fluoro-methyl-benzene [1-Fluoro-2-methyl-benzene]	C7.H7.F	95-52-3	10	1	3	3	3	1
92		Carbonochloridothioic acid, S-methyl ester	C2.H3.O.S.CL	2812-72-8	5	0	1	1	0	3
93		1,1-Dichloro-ethene	C2.H2.CL2	75-35-4	1	0	0	0	0	1
94		4-Chloro-2-(phenylmethyl)-phenol	C13.H11.O.CL	120-32-1	4	0	0	3	1	0
95	Organo-Silicon	1-Butynyl-trimethyl silane	C7.H14.SI	62108-37-6	7	0	2	1	3	1
96		Trimethyl[(1-methyl-2-propynyl)oxy]-silane	C7.H14.O.SI	17869-76-0	5	0	2	0	3	0

(a) Tentative compound identification is based on search vs. the NBS mass spectral library. Confirmation has not been achieved by comparing retention with an authentic standard. In cases where more than one reference compound successfully matched the unknown spectrum, a general descriptive name is reported and the best ranked NBS name is provided in brackets.

(b) In cases where both a general name and an NBS name is reported, the formula corresponds to the NBS name and may not be applicable to the general name.

(c) In cases where both a general name and an NBS name is reported, the CAS no. corresponds to the NBS name.

Table 7. Unidentified Peaks in the Volatile Organic Analysis Data Set vs. Frequency/Census Region

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region			
			North Central	Northeast	South	West
I.S.	1.000	46	12	9	19	6
1	.481	46	12	9	19	6
2	3.216	46	12	9	19	6
3	3.114	45	11	9	19	6
4	2.659	44	12	9	18	5
5	4.213	43	11	9	17	6
6	.370	41	9	9	18	5
7	2.398	41	11	8	18	4
8	.405	34	11	8	12	3
9	2.890	30	8	6	11	5
10	4.353	28	4	9	10	5
11	3.862	24	6	6	12	0
12	.286	23	5	3	12	3
13	3.322	21	10	4	5	2
14	3.314	18	7	4	6	1
15	2.771	14	4	2	7	1
16	2.689	13	5	1	5	2
17	1.997	12	2	6	3	1
18	3.384	12	3	0	9	0
19	3.873	12	1	2	7	2
20	2.666	11	3	1	6	1
21	4.390	11	2	2	4	3
22	2.570	10	2	1	5	2
23	3.962	9	0	1	7	1
24	4.142	9	4	0	5	0
25	.335	8	1	1	6	0
26	2.369	8	1	2	4	1
27	2.619	8	2	2	3	1
28	3.364	8	1	4	3	0
29	3.812	8	2	4	1	1
30	1.488	7	1	0	6	0
31	2.572	7	4	0	2	1
32	3.177	7	2	3	2	0
33	4.159	7	1	0	4	2
34	2.053	6	3	2	1	0
35	4.388	6	1	2	3	0
36	4.573	6	3	3	0	0
37	.802	5	1	4	0	0
38	1.744	5	0	2	1	2
39	2.495	5	2	1	2	0
40	2.867	5	2	2	0	1
41	2.906	5	1	1	2	1
42	3.308	5	4	0	0	1
43	3.501	5	0	0	5	0
44	4.319	5	2	1	2	0
45	.277	4	2	1	1	0
46	.408	4	0	0	2	2

Table 7 (continued)

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region			
			North Central	Northeast	South	West
47	1.719	4	1	0	2	1
48	3.064	4	0	0	2	2
49	3.159	4	2	0	2	0
50	3.513	4	3	1	0	0
51	3.881	4	2	0	1	1
52	3.908	4	0	3	1	0
53	4.317	4	0	0	3	1
54	.381	3	2	0	1	0
55	1.141	3	2	0	0	1
56	2.721	3	2	0	0	1
57	3.482	3	1	0	1	1
58	4.146	3	2	0	1	0
59	.285	2	2	0	0	0
60	.573	2	1	0	0	1
61	2.141	2	2	0	0	0
62	2.892	2	0	0	2	0
63	3.012	2	1	0	0	1
64	3.551	2	0	0	1	1
65	3.564	2	2	0	0	0
66	3.700	2	1	0	1	0
67	3.963	2	0	1	0	1
68	4.113	2	0	0	2	0
69	.313	1	1	0	0	0
70	1.036	1	1	0	0	0
71	1.511	1	0	0	0	1
72	1.672	1	1	0	0	0
73	2.028	1	0	1	0	0
74	2.239	1	1	0	0	0
75	2.262	1	0	0	1	0
76	2.271	1	0	0	1	0
77	2.301	1	1	0	0	0
78	2.407	1	1	0	0	0
79	2.671	1	0	0	0	1
80	2.891	1	0	0	0	1
81	2.907	1	0	1	0	0
82	2.988	1	1	0	0	0
83	3.073	1	0	0	1	0
84	3.100	1	0	0	1	0
85	3.175	1	0	0	1	0
86	3.314	1	0	0	1	0
87	3.371	1	0	0	1	0
88	3.453	1	1	0	0	0
89	3.461	1	1	0	0	0
90	3.494	1	1	0	0	0
91	3.650	1	0	0	1	0
92	3.782	1	0	1	0	0
93	3.829	1	1	0	0	0

Table 7 (concluded)

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region			
			North Central	Northeast	South	West
94	3.975	1	0	0	1	0
95	3.993	1	0	0	1	0
96	4.192	1	0	1	0	0
97	4.635	1	0	1	0	0
98	4.812	1	0	1	0	0
99	5.004	1	0	1	0	0

Table 8. Unidentified Peaks in the 6% Florisil Semivolatile Organic Analysis Data Set vs. Frequency/Census Region

Index	Average RRT	Total Number of Occurences	Number of Occurrences in Each Region				Number of Occurences in Blanks
			North Central	Northeast	South	West	
IS	1.000	44	12	9	18	5	3
1	0.924	42	12	9	18	3	0
2	1.600	42	12	7	18	5	2
3	0.759	38	10	9	17	2	0
4	1.027	38	12	8	13	5	0
5	1.023	35	9	6	16	4	0
6	1.117	34	12	3	15	4	0
7	1.706	34	11	5	16	2	1
8	1.129	32	12	1	15	4	0
9	0.879	31	10	6	14	1	0
10	0.702	30	9	4	13	4	0
11	0.919	30	9	7	12	2	0
12	0.990	29	9	4	13	3	0
13	0.838	28	8	4	13	3	0
14	0.912	26	6	5	11	4	0
15	1.481	26	9	1	14	2	2
16	1.760	25	7	2	14	2	1
17	0.985	24	7	5	10	2	0
18	1.059	24	8	1	12	3	0
19	0.673	23	6	6	8	3	0
20	0.993	23	5	6	10	2	0
21	0.982	22	8	3	9	2	0
22	1.533	22	8	2	11	1	1
23	1.063	21	6	4	8	3	0
24	1.199	21	9	3	9	0	0
25	1.374	21	6	3	11	1	1
26	0.726	19	7	3	8	1	0
27	1.741	19	6	3	9	1	0
28	0.952	17	7	2	6	2	0
29	1.237	17	6	1	7	3	0
30	1.629	17	3	2	11	1	2
31	1.586	16	6	1	9	0	1
32	0.493	15	3	5	4	3	0
33	1.002	15	5	2	7	1	0
34	1.065	15	4	2	8	1	0
35	0.839	14	3	3	7	1	0
36	1.070	14	4	1	6	3	0
37	1.728	14	6	1	6	1	0
38	0.574	13	2	0	9	2	0
39	0.665	13	6	2	5	0	0
40	1.178	13	5	0	7	1	0
41	1.280	13	5	1	6	1	0
42	1.297	13	4	0	8	1	0
43	0.190	12	3	3	4	2	0
44	0.666	12	5	4	2	1	0
45	0.310	11	4	2	2	3	0
46	0.603	11	1	1	8	1	0
47	1.082	11	3	0	5	3	0
48	1.131	11	2	3	4	2	0
49	1.146	11	3	2	3	3	0
50	0.411	10	3	1	3	3	0

Table 8 (continued)

Index	Average RRT	Total Number of Occurences	Number of Occurrences in Each Region				Number of Occurences in Blanks
			North Central	Northeast	South	West	
51	0.780	10	2	1	5	2	0
52	1.009	10	2	0	5	3	0
53	1.160	10	4	2	3	1	0
54	1.219	10	4	2	3	1	0
55	1.224	9	4	2	1	2	0
56	0.220	8	2	3	1	2	0
57	0.670	8	0	1	6	1	0
58	0.959	8	4	1	2	1	0
59	1.178	8	2	1	4	1	0
60	1.197	8	0	1	5	2	0
61	1.626	8	3	1	4	0	0
62	1.638	8	4	0	4	0	0
63	0.360	7	2	0	4	1	0
64	0.674	7	1	4	2	0	0
65	0.897	7	1	0	6	0	0
66	0.932	7	2	2	3	0	0
67	1.051	7	3	1	1	2	0
68	1.094	7	4	1	2	0	0
69	1.427	7	1	1	4	1	1
70	1.475	7	1	5	1	0	0
71	1.681	7	4	1	1	1	0
72	1.773	7	2	2	3	0	0
73	0.337	6	1	0	4	1	0
74	0.662	6	1	2	1	2	0
75	0.880	6	1	1	2	2	0
76	1.177	6	4	0	2	0	0
77	1.253	6	3	0	2	1	0
78	1.681	6	1	1	4	0	2
79	0.278	5	0	3	2	0	0
80	0.472	5	2	0	3	0	0
81	0.736	5	2	0	3	0	0
82	0.991	5	3	0	2	0	0
83	1.057	5	3	0	1	1	0
84	1.069	5	2	2	1	0	0
85	1.073	5	1	2	1	1	0
86	1.085	5	2	2	1	0	0
87	1.195	5	0	0	3	2	0
88	1.407	5	3	0	2	0	0
89	0.399	4	0	4	0	0	0
90	0.661	4	3	0	1	0	0
91	0.730	4	1	0	2	1	0
92	0.965	4	0	3	1	0	2
93	1.068	4	2	0	1	1	0
94	1.144	4	2	1	1	0	0
95	1.195	4	2	0	1	1	0
96	1.222	4	1	0	2	1	0
97	1.326	4	1	1	0	2	0
98	1.355	4	2	0	2	0	0
99	1.389	4	2	0	2	0	0
100	1.411	4	2	0	2	0	0
101	1.538	4	1	1	1	1	0

Table 8 (continued)

Index	Average RRT	Total Number of Occurences	Number of Occurrences in Each Region				Number of Occurences in Blanks
			North Central	Northeast	South	West	
102	0.316	3	1	1	0	1	0
103	0.608	3	1	0	1	1	0
104	0.662	3	0	0	2	1	0
105	0.747	3	0	2	0	1	0
106	0.754	3	3	0	0	0	0
107	0.855	3	0	0	1	2	0
108	0.893	3	0	0	3	0	0
109	0.918	3	1	0	2	0	0
110	0.967	3	3	0	0	0	0
111	1.019	3	1	2	0	0	0
112	1.025	3	0	1	2	0	0
113	1.041	3	1	2	0	0	0
114	1.045	3	1	0	2	0	0
115	1.050	3	0	1	1	1	0
116	1.055	3	2	0	1	0	0
117	1.076	3	3	0	0	0	0
118	1.107	3	0	3	0	0	0
119	1.109	3	0	0	3	0	0
120	1.186	3	0	1	1	1	0
121	1.244	3	0	0	3	0	0
122	1.251	3	1	0	2	0	0
123	1.414	3	0	1	1	1	0
124	1.457	3	0	0	3	0	0
125	1.585	3	0	0	3	0	0
126	0.325	2	1	0	1	0	0
127	0.356	2	0	2	0	0	0
128	0.747	2	0	2	0	0	0
129	0.754	2	0	0	2	0	0
130	0.817	2	1	0	0	1	0
131	0.823	2	0	2	0	0	0
132	0.855	2	0	0	1	1	0
133	0.896	2	0	1	0	1	0
134	0.898	2	0	2	0	0	0
135	0.905	2	0	2	0	0	0
136	0.933	2	0	0	1	1	0
137	0.976	2	0	0	2	0	0
138	0.982	2	2	0	0	0	0
139	0.985	2	0	0	1	1	0
140	1.020	2	2	0	0	0	0
141	1.038	2	1	0	1	0	0
142	1.053	2	0	0	2	0	0
143	1.080	2	1	0	1	0	0
144	1.106	2	0	1	0	1	0
145	1.120	2	0	2	0	0	0
146	1.124	2	1	0	1	0	0
147	1.143	2	2	0	0	0	0
148	1.152	2	0	0	1	1	0
149	1.158	2	0	1	1	0	0
150	1.179	2	0	1	0	1	0
151	1.221	2	0	0	2	0	0
152	1.252	2	0	0	2	0	0

Table 8 (continued)

Index	Average RRT	Total Number of Occurences	Number of Occurrences in Each Region				Number of Occurences in Blanks
			North Central	Northeast	South	West	
153	1.336	2	2	0	0	0	0
154	1.345	2	0	0	2	0	0
155	1.360	2	1	1	0	0	0
156	1.382	2	1	0	1	0	0
157	1.542	2	0	0	2	0	0
158	1.577	2	2	0	0	0	0
159	1.589	2	0	1	1	0	0
160	1.600	2	0	1	0	1	0
161	1.680	2	0	0	2	0	0
162	1.727	2	1	1	0	0	1
163	1.731	2	1	0	1	0	0
164	0.229	1	0	1	0	0	0
165	0.255	1	0	1	0	0	0
166	0.266	1	0	1	0	0	0
167	0.269	1	0	0	0	1	0
168	0.279	1	0	0	0	1	0
169	0.293	1	1	0	0	0	0
170	0.300	1	0	1	0	0	0
171	0.329	1	1	0	0	0	0
172	0.357	1	0	0	0	1	0
173	0.406	1	1	0	0	0	0
174	0.406	1	1	0	0	0	0
175	0.463	1	0	1	0	0	0
176	0.499	1	0	0	1	0	0
177	0.539	1	0	0	0	1	0
178	0.575	1	0	1	0	0	0
179	0.672	1	0	0	1	0	0
180	0.676	1	0	0	1	0	0
181	0.708	1	0	0	1	0	0
182	0.724	1	1	0	0	0	0
183	0.732	1	1	0	0	0	0
184	0.732	1	0	0	0	1	0
185	0.734	1	0	1	0	0	0
186	0.742	1	0	0	1	0	0
187	0.743	1	0	0	1	0	0
188	0.747	1	0	0	1	0	0
189	0.749	1	1	0	0	0	0
190	0.799	1	1	0	0	0	0
191	0.829	1	0	1	0	0	0
192	0.830	1	1	0	0	0	0
193	0.855	1	1	0	0	0	0
194	0.892	1	0	1	0	0	0
195	0.911	1	0	1	0	0	2
196	0.914	1	1	0	0	0	0
197	0.973	1	1	0	0	0	0
198	1.011	1	1	0	0	0	0
199	1.018	1	0	0	1	0	0
200	1.035	1	0	0	1	0	0
201	1.051	1	0	0	1	0	0
202	1.053	1	0	1	0	0	0
203	1.060	1	0	0	1	0	0

Table 8 (continued)

Index	Average RRT	Total Number of Occurences	Number of Occurrences in Each Region				Number of Occurences in Blanks
			North Central	Northeast	South	West	
204	1.064	1	0	1	0	0	0
205	1.075	1	1	0	0	0	0
206	1.078	1	0	0	0	1	0
207	1.084	1	1	0	0	0	0
208	1.107	1	0	0	1	0	0
209	1.117	1	0	1	0	0	0
210	1.117	1	0	0	1	0	0
211	1.118	1	0	0	1	0	0
212	1.121	1	0	0	1	0	0
213	1.122	1	0	0	1	0	0
214	1.134	1	0	0	0	1	0
215	1.134	1	0	1	0	0	0
216	1.138	1	1	0	0	0	0
217	1.140	1	0	0	1	0	0
218	1.140	1	0	0	1	0	0
219	1.152	1	1	0	0	0	0
220	1.161	1	0	1	0	0	0
221	1.170	1	1	0	0	0	0
222	1.189	1	0	0	1	0	0
223	1.208	1	0	1	0	0	0
224	1.217	1	1	0	0	0	0
225	1.226	1	0	1	0	0	0
226	1.262	1	0	0	1	0	0
227	1.288	1	1	0	0	0	0
228	1.289	1	0	0	1	0	0
229	1.304	1	0	1	0	0	0
230	1.348	1	0	0	1	0	0
231	1.349	1	0	0	1	0	0
232	1.349	1	1	0	0	0	0
233	1.350	1	1	0	0	0	0
234	1.356	1	1	0	0	0	0
235	1.375	1	1	0	0	0	0
236	1.379	1	0	0	1	0	0
237	1.394	1	1	0	0	0	0
238	1.407	1	0	0	1	0	0
239	1.534	1	0	0	1	0	0
240	1.588	1	0	0	1	0	0
241	1.590	1	0	1	0	0	0
242	1.596	1	0	0	1	0	0
243	1.624	1	1	0	0	0	0
244	1.634	1	0	0	1	0	0
245	1.646	1	0	0	1	0	0
246	1.659	1	0	0	1	0	0
247	1.676	1	0	1	0	0	0
248	1.678	1	0	1	0	0	0
249	1.701	1	0	0	1	0	0
250	1.709	1	0	0	1	0	0
251	1.718	1	0	1	0	0	1
252	1.721	1	0	0	1	0	0
253	1.731	1	0	0	1	0	0
254	1.734	1	0	1	0	0	0

Table 8 (concluded)

Index	Average RRT	Total Number of Occurences	Number of Occurrences in Each Region				Number of Occurences in Blanks
			North Central	Northeast	South	West	
255	1.734	1	0	1	0	0	0
256	1.740	1	0	0	1	0	0
257	1.804	1	1	0	0	0	0
258	1.889	1	0	0	1	0	0

Table 9. Unidentified Peaks in the 15/50% Florisil Semivolatile Organic Analysis Data Set vs. Frequency/Census Region

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region				Number of Occurrences in Blanks
			North Central	Northeast	South	West	
I.S.	1.000	46	12	9	19	6	4
1	1.920	44	12	9	18	5	1
2	0.419	42	11	9	17	5	3
3	1.052	41	12	6	18	5	0
4	1.007	40	12	5	18	5	0
5	0.452	38	11	6	15	6	3
6	1.616	38	12	6	17	3	1
7	0.402	37	10	7	14	6	3
8	0.633	35	9	9	13	4	0
9	1.742	35	11	6	16	2	0
10	0.449	34	10	6	12	6	3
11	1.569	34	10	5	16	3	1
12	2.034	34	10	5	14	5	1
13	1.692	33	11	4	16	2	0
14	1.682	32	10	7	14	1	0
15	1.710	32	11	3	16	2	0
16	0.437	29	6	7	10	6	3
17	0.606	29	7	6	11	5	0
18	1.238	29	12	2	13	2	0
19	1.657	28	10	6	10	2	1
20	1.187	28	9	3	14	2	0
21	1.453	28	11	4	11	2	0
22	0.839	27	10	3	12	2	0
23	1.665	27	10	3	13	1	0
24	0.647	26	7	4	12	3	0
25	1.128	26	11	0	14	1	0
26	2.059	26	9	2	13	2	0
27	1.953	25	6	4	13	2	1
28	1.440	25	8	3	13	1	0
29	1.490	24	8	3	11	2	0
30	1.722	23	8	4	9	2	0
31	1.430	22	7	3	11	1	0
32	0.932	21	7	1	12	1	0
33	1.115	21	8	0	11	2	0
34	1.223	21	6	3	9	3	0
35	2.009	20	6	2	10	2	1
36	0.589	20	5	5	5	5	0
37	1.147	20	5	0	13	2	0
38	1.567	20	6	3	9	2	0
39	1.235	19	6	1	11	1	0
40	1.178	18	5	3	9	1	1
41	0.555	18	2	6	8	2	0
42	0.990	17	7	1	9	0	0
43	1.319	17	6	2	8	1	0
44	1.629	16	5	3	7	1	2
45	0.876	16	4	2	8	2	0
46	0.680	15	3	2	7	3	0
47	0.912	15	6	0	8	1	0
48	1.086	15	5	1	6	3	0
49	1.089	15	6	2	6	1	0
50	1.556	15	5	3	5	2	0
51	1.980	15	4	2	8	1	0
52	1.929	14	3	1	8	2	1
53	0.982	14	6	1	7	0	0
54	1.809	14	3	2	8	1	0
55	1.027	13	6	0	6	1	0
56	1.210	13	5	3	4	1	0
57	1.500	13	4	3	5	1	0
58	1.950	13	4	2	6	1	0
59	0.586	12	4	0	7	1	1
60	0.858	12	5	3	4	0	1
61	1.511	12	4	3	4	1	0
62	1.961	12	5	1	5	1	0
63	2.014	12	4	0	6	2	0

Table 9 (continued)

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region				Number of Occurrences in Blanks
			North Central	Northeast	South	West	
64	2.088	12	4	2	5	1	0
65	0.996	11	2	3	5	1	1
66	1.027	11	2	3	5	1	1
67	0.218	11	2	3	4	2	0
68	0.398	11	3	2	6	0	0
69	1.475	11	4	3	4	0	0
70	1.522	11	3	2	4	2	0
71	1.542	11	3	2	5	1	0
72	1.980	11	4	1	5	1	0
73	0.745	10	3	1	6	0	0
74	0.904	10	3	1	5	1	0
75	1.105	10	2	3	4	1	0
76	1.359	10	3	3	4	0	0
77	0.429	9	5	1	2	1	0
78	0.673	9	4	2	3	0	0
79	0.897	9	2	1	5	1	0
80	1.548	9	3	2	3	1	0
81	1.989	9	4	0	5	0	0
82	0.226	8	2	2	2	2	0
83	0.243	8	2	2	2	2	0
84	0.989	8	4	0	3	1	0
85	1.149	8	3	2	3	0	0
86	1.351	8	4	0	3	1	0
87	1.973	8	4	0	4	0	0
88	2.151	8	2	1	4	1	0
89	2.174	8	2	1	5	0	0
90	0.301	7	2	0	2	3	0
91	0.392	7	2	1	3	1	0
92	0.520	7	0	6	0	1	0
93	0.672	7	1	0	5	1	0
94	1.198	7	2	0	5	0	0
95	1.675	7	2	0	4	1	0
96	1.889	7	1	2	3	1	0
97	0.492	6	3	2	0	1	0
98	0.758	6	3	1	2	0	0
99	1.175	6	3	0	3	0	0
100	1.202	6	1	0	4	1	0
101	1.308	6	1	2	3	0	0
102	1.472	6	1	0	3	2	0
103	1.531	6	3	0	3	0	0
104	1.966	6	1	2	3	0	0
105	2.137	6	1	1	3	1	0
106	1.531	5	1	0	3	1	1
107	0.374	5	1	1	2	1	0
108	0.450	5	1	2	2	0	0
109	0.540	5	1	0	4	0	0
110	0.547	5	1	1	3	0	0
111	0.559	5	1	1	3	0	0
112	0.573	5	1	0	3	1	0
113	0.762	5	2	0	3	0	0
114	0.918	5	3	0	2	0	0
115	1.062	5	0	1	3	1	0
116	1.070	5	2	0	2	1	0
117	1.105	5	1	2	2	0	0
118	1.138	5	3	0	2	0	0
119	1.175	5	2	3	0	0	0
120	1.288	5	0	2	2	1	0
121	1.460	5	1	1	2	1	0
122	1.716	5	1	1	3	0	0
123	1.729	5	2	1	2	0	0
124	0.475	4	1	1	1	1	0
125	0.507	4	0	1	3	0	0
126	0.520	4	0	1	2	1	0
127	0.667	4	3	0	1	0	0

Table 9 (continued)

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region				Number of Occurrences in Blanks
			North Central	Northeast	South	West	
128	0.721	4	0	0	4	0	0
129	0.832	4	0	0	4	0	0
130	0.936	4	1	1	1	1	0
131	1.061	4	1	1	2	0	0
132	1.109	4	2	1	0	1	0
133	1.153	4	0	2	2	0	0
134	1.173	4	2	0	2	0	0
135	1.277	4	1	1	2	0	0
136	1.328	4	0	0	4	0	0
137	1.580	4	2	1	0	1	0
138	1.927	4	2	0	1	1	0
139	1.979	4	1	1	1	1	0
140	2.000	4	2	0	2	0	0
141	0.319	3	2	0	1	0	1
142	0.375	3	1	1	0	1	1
143	0.609	3	1	0	2	0	1
144	0.307	3	0	0	2	1	0
145	0.346	3	1	1	1	0	0
146	0.353	3	0	0	0	3	0
147	0.487	3	1	0	2	0	0
148	0.727	3	0	0	3	0	0
149	0.739	3	1	1	0	1	0
150	0.790	3	0	2	0	1	0
151	0.821	3	0	1	2	0	0
152	0.828	3	0	1	2	0	0
153	1.083	3	0	0	3	0	0
154	1.119	3	1	0	2	0	0
155	1.123	3	2	0	1	0	0
156	1.195	3	0	0	3	0	0
157	1.309	3	0	0	2	1	0
158	1.404	3	1	1	1	0	0
159	1.448	3	0	1	2	0	0
160	1.538	3	1	0	2	0	0
161	1.856	3	2	0	1	0	0
162	1.953	3	2	0	1	0	0
163	2.084	3	2	0	1	0	0
164	2.091	3	1	0	2	0	0
165	0.512	2	2	0	0	0	1
166	0.572	2	0	0	2	0	1
167	1.809	2	0	0	2	0	1
168	1.900	2	0	0	2	0	1
169	0.237	2	1	0	1	0	0
170	0.261	2	0	2	0	0	0
171	0.337	2	1	0	1	0	0
172	0.341	2	0	2	0	0	0
173	0.342	2	1	0	1	0	0
174	0.382	2	0	0	1	1	0
175	0.413	2	0	0	2	0	0
176	0.435	2	1	0	0	1	0
177	0.450	2	1	0	1	0	0
178	0.489	2	0	0	2	0	0
179	0.496	2	0	0	2	0	0
180	0.552	2	1	0	1	0	0
181	0.599	2	0	2	0	0	0
182	0.614	2	0	2	0	0	0
183	0.677	2	0	2	0	0	0
184	0.758	2	1	0	0	1	0
185	0.791	2	1	0	1	0	0
186	0.908	2	1	0	1	0	0
187	0.921	2	0	0	2	0	0
188	0.957	2	1	0	1	0	0
189	1.059	2	1	0	1	0	0
190	1.261	2	1	0	1	0	0
191	1.283	2	0	1	1	0	0

Table 9 (continued)

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region				Number of Occurrences in Blanks
			North Central	Northeast	South	West	
192	1.291	2	0	0	2	0	0
193	1.297	2	1	0	1	0	0
194	1.353	2	1	0	1	0	0
195	1.463	2	1	1	0	0	0
196	1.507	2	0	1	1	0	0
197	1.516	2	0	1	1	0	0
198	1.525	2	1	1	0	0	0
199	1.586	2	1	0	1	0	0
200	1.594	2	2	0	0	0	0
201	1.673	2	2	0	0	0	0
202	1.866	2	0	1	1	0	0
203	1.931	2	1	0	1	0	0
204	2.030	2	1	0	1	0	0
205	2.102	2	0	0	1	1	0
206	0.333	1	0	1	0	0	1
207	0.544	1	0	0	1	0	1
208	0.199	1	0	0	1	0	0
209	0.203	1	0	0	1	0	0
210	0.216	1	0	1	0	0	0
211	0.221	1	0	1	0	0	0
212	0.239	1	0	0	1	0	0
213	0.240	1	0	0	1	0	0
214	0.241	1	1	0	0	0	0
215	0.254	1	1	0	0	0	0
216	0.266	1	0	0	1	0	0
217	0.268	1	0	0	1	0	0
218	0.283	1	0	1	0	0	0
219	0.285	1	0	1	0	0	0
220	0.293	1	1	0	0	0	0
221	0.300	1	0	1	0	0	0
222	0.327	1	1	0	0	0	0
223	0.344	1	0	0	0	1	0
224	0.352	1	0	0	1	0	0
225	0.353	1	0	0	0	1	0
226	0.358	1	0	0	0	1	0
227	0.359	1	0	1	0	0	0
228	0.362	1	0	0	0	1	0
229	0.365	1	0	1	0	0	0
230	0.370	1	0	1	0	0	0
231	0.371	1	0	0	0	1	0
232	0.372	1	0	0	1	0	0
233	0.394	1	0	0	1	0	0
234	0.405	1	0	0	1	0	0
235	0.414	1	0	0	1	0	0
236	0.419	1	0	1	0	0	0
237	0.421	1	0	0	1	0	0
238	0.422	1	0	0	1	0	0
239	0.455	1	0	0	1	0	0
240	0.463	1	1	0	0	0	0
241	0.465	1	0	1	0	0	0
242	0.504	1	0	0	0	1	0
243	0.507	1	0	0	0	1	0
244	0.510	1	0	1	0	0	0
245	0.516	1	0	0	1	0	0
246	0.545	1	0	0	1	0	0
247	0.575	1	0	0	1	0	0
248	0.584	1	0	0	0	1	0
249	0.652	1	0	0	1	0	0
250	0.653	1	0	1	0	0	0
251	0.678	1	0	0	1	0	0
252	0.683	1	0	1	0	0	0
253	0.711	1	1	0	0	0	0
254	0.744	1	0	0	0	1	0
255	0.745	1	0	0	1	0	0

Table 9 (continued)

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region				Number of Occurrences in Blanks
			North Central	Northeast	South	West	
256	0.767	1	1	0	0	0	0
257	0.771	1	0	0	1	0	0
258	0.775	1	0	0	1	0	0
259	0.779	1	0	0	1	0	0
260	0.786	1	0	0	1	0	0
261	0.787	1	0	0	1	0	0
262	0.821	1	0	0	0	1	0
263	0.915	1	0	0	1	0	0
264	0.929	1	0	0	1	0	0
265	0.945	1	0	0	1	0	0
266	0.960	1	0	0	1	0	0
267	0.988	1	0	0	1	0	0
268	1.017	1	0	1	0	0	0
269	1.018	1	0	0	1	0	0
270	1.037	1	0	0	1	0	0
271	1.046	1	0	0	1	0	0
272	1.061	1	1	0	0	0	0
273	1.063	1	0	0	1	0	0
274	1.070	1	0	0	1	0	0
275	1.089	1	0	0	1	0	0
276	1.091	1	0	0	1	0	0
277	1.112	1	0	0	1	0	0
278	1.121	1	0	0	1	0	0
279	1.140	1	1	0	0	0	0
280	1.174	1	0	0	0	1	0
281	1.180	1	0	0	1	0	0
282	1.197	1	0	0	1	0	0
283	1.204	1	0	0	1	0	0
284	1.204	1	0	0	1	0	0
285	1.218	1	0	0	1	0	0
286	1.223	1	0	0	1	0	0
287	1.226	1	0	0	1	0	0
288	1.243	1	0	0	1	0	0
289	1.248	1	0	0	1	0	0
290	1.289	1	1	0	0	0	0
291	1.291	1	0	0	1	0	0
292	1.296	1	0	0	1	0	0
293	1.309	1	0	0	1	0	0
294	1.311	1	0	0	1	0	0
295	1.335	1	0	0	1	0	0
296	1.342	1	1	0	0	0	0
297	1.346	1	0	0	1	0	0
298	1.348	1	0	0	1	0	0
299	1.350	1	0	0	1	0	0
300	1.363	1	0	0	1	0	0
301	1.366	1	0	0	1	0	0
302	1.377	1	0	0	1	0	0
303	1.384	1	0	0	1	0	0
304	1.386	1	0	0	1	0	0
305	1.390	1	0	0	1	0	0
306	1.403	1	0	0	1	0	0
307	1.421	1	0	1	0	0	0
308	1.422	1	1	0	0	0	0
309	1.427	1	0	0	1	0	0
310	1.433	1	1	0	0	0	0
311	1.435	1	1	0	0	0	0
312	1.457	1	0	0	1	0	0
313	1.481	1	1	0	0	0	0
314	1.492	1	0	0	1	0	0
315	1.495	1	1	0	0	0	0
316	1.499	1	1	0	0	0	0
317	1.523	1	1	0	0	0	0
318	1.525	1	0	0	1	0	0
319	1.531	1	1	0	0	0	0

Table 9 (concluded)

Index	Average RRT	Total Number of Occurrences	Number of Occurrences in Each Region				Number of Occurrences in Blanks
			North Central	Northeast	South	West	
320	1.545	1	1	0	0	0	0
321	1.562	1	1	0	0	0	0
322	1.583	1	1	0	0	0	0
323	1.584	1	1	0	0	0	0
324	1.589	1	1	0	0	0	0
325	1.596	1	1	0	0	0	0
326	1.602	1	1	0	0	0	0
327	1.606	1	1	0	0	0	0
328	1.607	1	1	0	0	0	0
329	1.671	1	0	0	1	0	0
330	1.695	1	0	0	1	0	0
331	1.740	1	0	1	0	0	0
332	1.761	1	0	0	1	0	0
333	1.762	1	0	0	1	0	0
334	1.776	1	1	0	0	0	0
335	1.839	1	1	0	0	0	0
336	1.907	1	0	0	1	0	0
337	1.964	1	0	0	1	0	0
338	1.973	1	0	0	1	0	0
339	1.980	1	1	0	0	0	0
340	1.991	1	0	0	1	0	0
341	2.053	1	0	0	1	0	0
342	2.063	1	0	0	1	0	0
343	2.107	1	1	0	0	0	0

Table 10. NHATS FY82 Composite Peak Inventory - Volatile Organic Analysis Data Set

Index	Sample Name	Number of Peaks Submitted to ACORN Program	Number of Compounds Identified by ACORN Program	Number of Unidentified Peaks Remaining	Number of Compounds Identified by Target Compound Analysis
1	1-EN-VO-0-14	68	48	20	23
2	1-EN-VO-15-44	63	42	21	23
3	1-EN-VO-45+	62	45	17	22
4	1-ES-VO-0-14	51	35	16	21
5	1-ES-VO-15-44	43	26	17	21
6	1-ES-VO-45+	49	35	14	21
7	1-MA-VO-0-14	61	42	19	23
8	1-MA-VO-15-44	54	35	19	24
9	1-MA-VO-45+	60	40	20	23
10	1-MO-VO-0-14	49	33	16	21
11	1-MO-VO-15-44	45	30	15	24
12	1-MO-VO-45+	50	32	18	22
13	1-NE-VO-0-14	48	36	12	22
14	1-NE-VO-15-44	53	35	18	23
15	1-NE-VO-45+	54	34	20	21
16	1-PA-VO-0-14	52	38	14	22
17	1-PA-VO-15-44	56	42	14	24
18	1-PA-VO-45+	68	47	21	23
19	1-SA-VO-0-14	56	41	15	21
20	1-SA-VO-15-44	58	39	19	23
21	1-SA-VO-45+	44	30	14	22
22	1-WN-VO-0-14	57	40	17	22
23	1-WN-VO-15-44	59	42	17	22
24	1-WN-VO-45+	70	46	24	24
25	1-WS-VO-0-14	54	36	18	20
26	1-WS-VO-15-44	61	43	18	20
27	1-WS-VO-45+	60	40	20	21
28	2-EN-VO-0-14	55	37	18	22
29	2-EN-VO-15-44	70	47	23	24
30	2-EN-VO-45+	68	49	19	22
31	2-ES-VO-15-44	59	40	19	25
32	2-ES-VO-45+	53	36	17	24
33	2-MA-VO-0-14	56	38	18	23
34	2-MA-VO-15-44	58	39	19	24
35	2-MA-VO-45+	52	32	20	22
36	2-SA-VO-0-14	58	39	19	22
37	2-SA-VO-15-44	59	43	16	24
38	2-SA-VO-45+	67	47	20	24
39	2-WN-VO-45+	45	31	14	22
40	2-WS-VO-15-44	64	42	22	24
41	3-EN-VO-15-44	59	43	16	23
42	3-EN-VO-45+	68	46	22	23
43	3-SA-VO-15-44	58	40	18	23
44	3-SA-VO-45+	62	42	20	23
45	4-SA-VO-15-44	53	38	15	21
46	4-SA-VO-45+	50	33	17	19

Table 11. NHATS FY82 Composite Peak Inventory - 6% Florisil Semivolatile Organic Analysis Data Set

Index	Sample Name	Number of Peaks Submitted to ACORN Program	Number of Compounds Identified by ACORN Program	Number of Unidentified Peaks Remaining	Number of Compounds Identified by Target Compound Analysis
1	1-EN-SVO-0-14	50	16	34	10
2	1-EN-SVO-15-44	63	19	44	19
3	1-EN-SVO-45+	79	21	58	14
4	1-ES-SVO-0-14	55	22	33	26
5	1-ES-SVO-15-44	50	24	26	34
6	1-ES-SVO-45+	54	26	28	22
7	1-MA-SVO-0-14	50	16	34	22
8	1-MA-SVO-15-44	36	13	23	28
9	1-MA-SVO-45+	54	26	28	21
10	1-MO-SVO-0-14	37	17	20	11
11	1-MO-SVO-15-44	66	23	43	15
12	1-MO-SVO-45+	64	23	41	23
13	1-NE-SVO-0-14	45	16	29	10
14	1-NE-SVO-15-44	31	14	17	23
15	1-NE-SVO-45+	82	28	54	19
16	1-PA-SVO-0-14	48	18	30	13
17	1-PA-SVO-45+	59	22	37	20
18	1-SA-SVO-0-14	79	34	45	23
19	1-SA-SVO-15-44	79	23	56	24
20	1-SA-SVO-45+	80	31	49	24
21	1-WN-SVO-0-14	55	14	41	20
22	1-WN-SVO-15-44	36	13	23	26
23	1-WN-SVO-45+	54	27	27	37
24	1-WS-SVO-0-14	54	14	40	15
25	1-WS-SVO-15-44	43	13	30	26
26	1-WS-SVO-45+	58	25	33	31
27	2-EN-SVO-0-14	49	14	35	14
28	2-EN-SVO-15-44	45	15	30	20
29	2-EN-SVO-45+	73	17	56	33
30	2-ES-SVO-45+	72	22	50	32
31	2-MA-SVO-0-14	46	17	29	23
32	2-MA-SVO-15-44	36	9	27	25
33	2-MA-SVO-45+	49	16	33	18
34	2-SA-SVO-0-14	59	16	43	13
35	2-SA-SVO-15-44	50	14	36	22
36	2-SA-SVO-45+	77	24	53	23
37	2-WN-SVO-45+	72	18	54	22
38	2-WS-SVO-15-44	46	13	33	16
39	3-EN-SVO-15-44	52	12	40	19
40	3-EN-SVO-45+	70	22	48	28
41	3-SA-SVO-15-44	50	14	36	33
42	3-SA-SVO-45+	59	27	31	30
43	4-SA-SVO-15-44	49	17	32	23
44	4-SA-SVO-45+	56	20	36	32

Table 12. NHATS FY82 Composite Peak Inventory - 15/50% Florisil Semivolatile Organic Analysis Data Set

Index	Sample Name	Number of Peaks Submitted to ACORN Program	Number of Compounds Identified by ACORN Program	Number of Unidentified Peaks Remaining	Number of Compounds Identified by Target Compound Analysis
1	1-EN-SVO-0-14	75	21	54	2
2	1-EN-SVO-15-44	67	20	47	1
3	1-EN-SVO-45+	60	19	41	2
4	1-ES-SVO-0-14	78	14	64	6
5	1-ES-SVO-15-44	68	15	53	7
6	1-ES-SVO-45+	91	18	73	1
7	1-MA-SVO-0-14	59	20	39	2
8	1-MA-SVO-15-44	33	12	21	4
9	1-MA-SVO-45+	41	21	20	3
10	1-MO-SVO-0-14	57	20	37	1
11	1-MO-SVO-15-44	75	19	56	3
12	1-MO-SVO-45+	79	16	63	4
13	1-NE-SVO-0-14	48	15	33	3
14	1-NE-SVO-15-44	24	11	13	3
15	1-NE-SVO-45+	58	24	34	3
16	1-PA-SVO-0-14	38	13	25	1
17	1-PA-SVO-15-44	38	13	25	1
18	1-PA-SVO-45+	57	16	41	3
19	1-SA-SVO-0-14	97	26	71	2
20	1-SA-SVO-15-44	68	20	48	2
21	1-SA-SVO-45+	94	29	65	3
22	1-WN-SVO-0-14	79	24	55	4
23	1-WN-SVO-15-44	60	12	48	4
24	1-WN-SVO-45+	91	27	64	5
25	1-WS-SVO-0-14	66	22	44	6
26	1-WS-SVO-15-44	68	16	52	5
27	1-WS-SVO-45+	96	23	73	6
28	2-EN-SVO-0-14	108	24	84	6
29	2-EN-SVO-15-44	73	15	58	7
30	2-EN-SVO-45+	102	21	81	6
31	2-ES-SVO-15-44	22	6	16	1
32	2-ES-SVO-45+	52	9	43	1
33	2-MA-SVO-0-14	83	21	62	4
34	2-MA-SVO-15-44	65	18	47	4
35	2-MA-SVO-45+	99	28	71	4
36	2-SA-SVO-0-14	88	24	64	5
37	2-SA-SVO-15-44	73	15	58	6
38	2-SA-SVO-45+	129	30	99	6
39	2-WN-SVO-45+	78	20	58	5
40	2-WS-SVO-15-44	79	20	59	3
41	3-EN-SVO-15-44	46	15	31	1
42	3-EN-SVO-45+	80	16	64	5
43	3-SA-SVO-15-44	57	14	43	5
44	3-SA-SVO-45+	77	18	59	2
45	4-SA-SVO-15-44	57	16	41	1
46	4-SA-SVO-45+	22	6	16	1

Each of the samples analyzed is identified under Sample Name. The sample name code includes a number to indicate the number of composites analyzed within a specific age group in a designated census division. For example, the code 1-EN-VO-14 indicates that this is the first composite from the East North Central (EN) census division representing the 0-14 age group. The code VO designates the composite was analyzed for volatile organic compounds. Each of the nine census divisions are represented in the tables (EN = East North Central; ES = East South Central; MA = Middle Atlantic; NE = New England; SA = South Atlantic; WN = West North Central; WS = West South Central; MO = Mountain; and PA = Pacific).

Additional tables detailing the frequency of occurrence of HRGC/MS responses are included in Appendices A through F, provided as a separate volume with this report. The information in these tables is identical to that provided in the previously described data tables (1 through 9). However, incidence of occurrence information is provided for the nine census divisions in addition to four census regions and three age groups. The tables in Appendices A through C are "dot matrix" tables displaying the incidence of occurrence of identified compounds for each of the samples analyzed in this study. Compound names are sorted in the same order as Tables 1 through 3. Sample data are arranged in a matrix of census region, census division, and age group. Each table in the appendices is devoted to a particular census region. The four census regions which are represented are the West, South, North Central, and Northeast.

Tables in Appendices D through F are "dot matrix" tables displaying the incidence of occurrence of unidentified compounds for each of the samples analyzed in this study. The tables in these appendices are organized identically to the tables in Appendices A through C.

V. DISCUSSION

This section provides a discussion of the limitations of the identification method and limitations of the FY82 data set.

A. Limitations of the Peak Identification Method

Discussions of the limitations to the peak identification method may be divided into two categories: limitations of the implementation of the method and limitations inherent to the method itself.

The primary concern regarding the implementation of the method was that it was not fully automated. A number of critical steps could have benefited from additional computer programming. The manual review process in particular was very time-consuming because all corrections to the seed library had to be made "by hand," i.e., an operator was required to make manual corrections to the summary report, identification list, and seed library. Spreadsheet generation also proved to be more time-consuming than originally anticipated. However, in spite of these limitations, the actual results of the procedure were not affected.

Inherent limitations of the identification scheme were more subtle. Certainly the most stringent limitation in this respect was the dependence of the program on high quality spectra. Unknown mass spectra with distinctive fragmentation patterns, acceptable signal strength, and no contamination from coeluting peaks were easily identified. Conversely, spectra with very little fragmentation, poor or excessive signal strength, or significant contamination were a constant problem.

This dependence upon quality mass spectra is not peculiar to this method. It is a necessary condition for the interpretation of mass spectra in general, whether automatic or manual. No method of automatic peak identification can be successful unless analytical conditions are optimzed for the generation of high quality mass spectra.

It should be emphasized that a manual review was performed for each compound tentatively identified in this report. In cases where identification to a specific compound isomer could not be conclusively determined, a non-specific compound or compound class name was reported. However, the full name of the best ranked NBS reference compound was also retained and reported in brackets.

B. Limitations of the FY82 Data

In addition to the limitations of the identification method described above, there were limitations with the FY82 adipose datafiles themselves when applied to the area of unknown peak identification. Most of these limitations stem from using GC/MS operating parameters which were optimized for target compound analysis rather than interpretation of unknown mass spectra. Three GC/MS operating parameters were identified which had an effect on the performance of the peak identification method: (1) sensitivity setting of the mass spectrometer; (2) mass scanning range of the mass spectrometer; and (3) temperature program rate of the HRGC. Background contribution also had an effect on the performance of the peak identification method. Each of these parameters is discussed below.

1. MS Sensitivity

The objective of the broad scan target compound analysis for the FY82 samples was to quantitate target compounds in the 50 to 100 ppb (ng/g) range. This sensitivity range is common in routine target compound analysis. Mass spectrometric response may be considered to be roughly proportional to concentration for a given sample type such as volatile or semivolatile. Also, the dynamic range of a mass spectrometer is approximately two orders of magnitude for quantitation and slightly higher for reliable mass spectral interpretation of unknown compounds. Spectra observed at sensitivities outside this range may not be adequate for identification purposes due to saturation at the high end and excessive noise or signal dropoff at the low end of the range. These estimates are quite general, with each compound having its own HRGC and MS performance characteristics.

Unfortunately, the organic matrix in the adipose samples of both the volatile and semivolatile data sets was very complex. At sensitivity

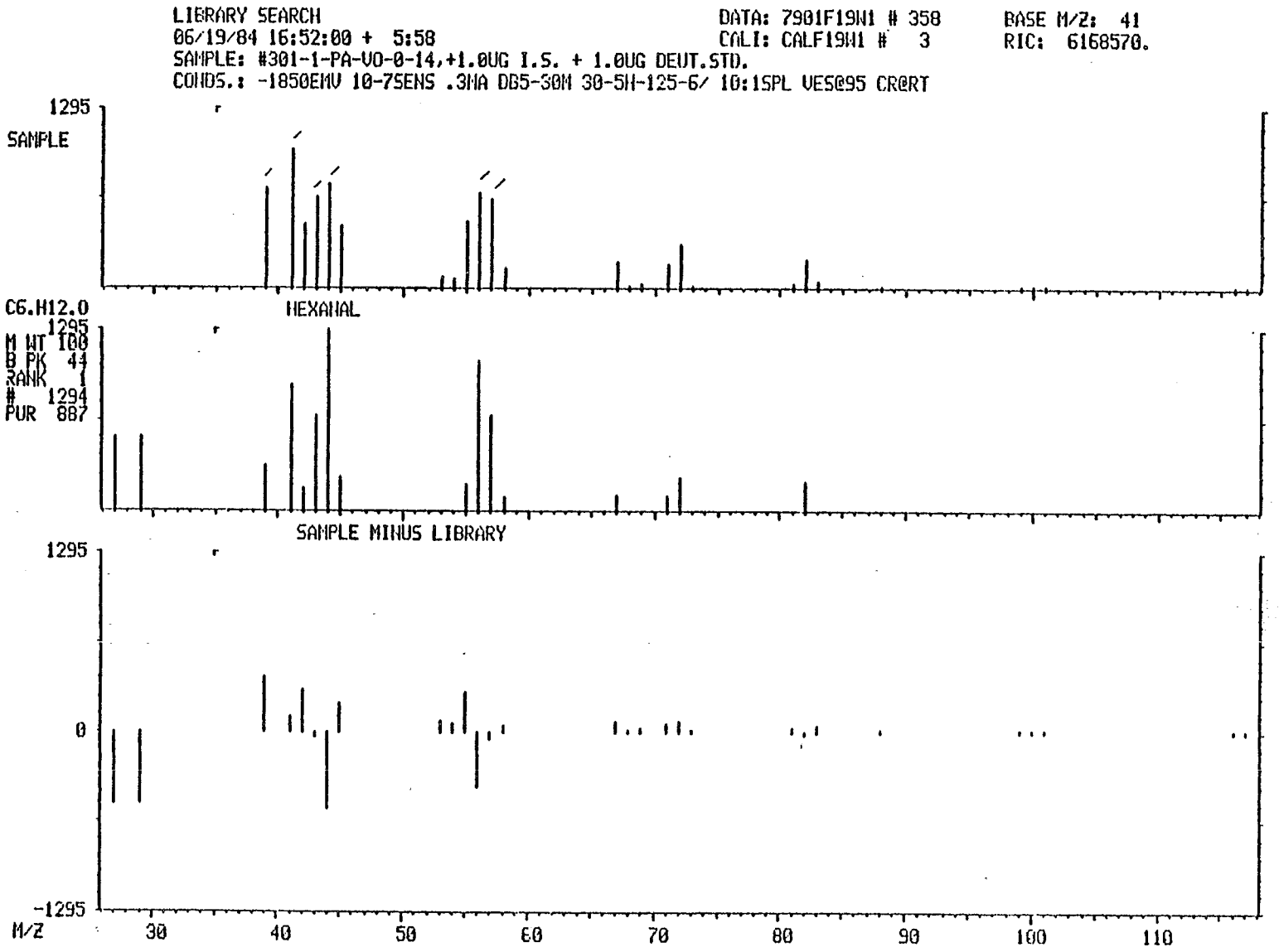

Figure 8. Example of degradation of mass spectral quality as a result of instrument saturation. The upper spectrum is taken from a peak which saturated the mass spectrometer. Tick marks above the mass histograms indicate ions which are saturated. The lower plot is the NBS reference mass spectrum for the compound.

settings required to keep the target compounds within the desired quantitation range, many unknown peaks had responses well outside the range necessary for reliable mass spectral interpretation. Figure 8 illustrates the effects of acquiring mass spectra at sensitivity settings inappropriate for mass spectral interpretation purposes. In this example, the results of an NBS library search of an unknown spectrum are shown. The mass spectrum at the top of the page shows the unknown spectrum. Tick marks above some of the masses indicate signal saturation. The spectrum immediately below the unknown spectrum is the best candidate chosen from the NBS library. Note that there is a marked change in the relative intensities of many of the saturated masses. Although in this case saturation did not prevent the NBS library search from choosing the correct candidate, other cases resulted in ACORN incorrectly identifying the unknown peak. Manual review of the data after each application of ACORN corrected these misassignments.

2. Scan Range Selection

The semivolatiles presented an additional problem which was related to the original MS operating parameters. The semivolatile samples were acquired using a mass range suitable for the detection of molecular clusters characteristic of chlorinated benzenes and polybrominated compounds such as polybrominated biphenyls. This required setting the mass spectrometer to scan in the high mass region (100-700 amu). A Finnigan/MAT 311A magnetic sector mass spectrometer was chosen for the analysis. Due to design constraints of magnetic mass spectrometers of this type, it was necessary to begin the mass scan at 100 amu in order to achieve an upper mass limit of 700 amu. Unfortunately, many compounds have significant mass fragmentation in the 30 to 100 amu mass range. Fragmentation in this low mass region is often of critical importance in correctly identifying a compound. Thus, the quality of semivolatile spectra was often marginal for reliable mass spectral interpretation purposes.

This problem was most acute for compounds with a molecular weight between 100 and 150 amu. In these cases there was often insufficient fragmentation to confirm the comparison with the NBS library. The effect of poor fragmentation on library search results is shown in Figure 9. The format of this output is identical to one shown previously in Figure 2. In this example, note that a number of compounds of varying elemental formulas were selected from the NBS library as likely candidates. However, the graphic comparison of the unknown to the three best candidates indicates that only one major peak at m/z 108 and three minor peaks clustered around the major peak were present in the unknown spectrum. It is also apparent from the graph that there is insufficient evidence to assign this spectrum to any of the candidates, as indicated by the close similarity of the unknown spectrum to the three best candidate spectra.

3. HRGC Temperature Program

The broad scan analysis of the FY82 composite samples was optimized for the most rapid turnaround time possible without sacrificing the quality of the target compound quantitation results. This was accomplished by using relatively fast GC temperature program rates (6°C/min for volatiles, 10°C/min

```
Library Search                    Data: 7901F13R1 # 179      Base m/z:   108
06/13/84 10:30:00 + 3:53          Call: CALF13R3 #   2      RIC:     229887.
Sample: 7901-8-052,6%,2-MA-SVO-0-14,1UL INJ (2UG D-10 ADDED)
Conds.: -1650EMV,70EV,1MA,DB5-30M-60-2H-310-10,45 SEC SPLITLESS

42222 spectra in LIBRARYNB searches for maximum PURITY
  438 matched at least 4 of the 11 largest peaks in the unknown
Reduction:   Pts/100 u :      40;  Windows:  50,  7
Pre-search:  Entries to pass: 200;  Sample peaks: 16
Main search: Masses:  99 - 550;  Norm int:  25;  Ratio factors:   2.0, 1.0

Rank In.      Name
1   1776 HYDRAZINE, PHENYL-
2   1778 1,3-BENZENEDIAMINE
3   6496 PYRIDINIUM, 1-AMINO-4-METHYL-, CHLORIDE
4   1891 1H-PYRROLE, 2,3,5-TRIMETHYL-
5   1775 1,2-BENZENEDIAMINE
6   7815 3-CYCLOPENTENE-1-ACETALDEHYDE, 2,2,3-TRIMETHYL-
7   1854 CYCLOPENTENE, 3-ETHYLIDENE-1-METHYL-
8   1782 PYRIMIDINE, 4,5-DIMETHYL-
9   1786 2-PYRIDINAMINE, 5-METHYL-

Rank  Formula          M.Wt  B.Pk   Purity   Fit   RFit
1     C6.H8.N2          108   108      948   967    948
2     C6.H8.N2          108   108      946   964    946
3     C6.H9.N2.CL       144    93      938   956    938
4     C7.H11.N          109   108      937   943    937
5     C6.H8.N2          108   108      924   938    924
6     C10.H16.O         152   108      922   940    981
7     C8.H12            108    93      920   934    920
8     C6.H8.N2          108   108      914   932    914
9     C6.H8.N2          108   108      847   864    847
```

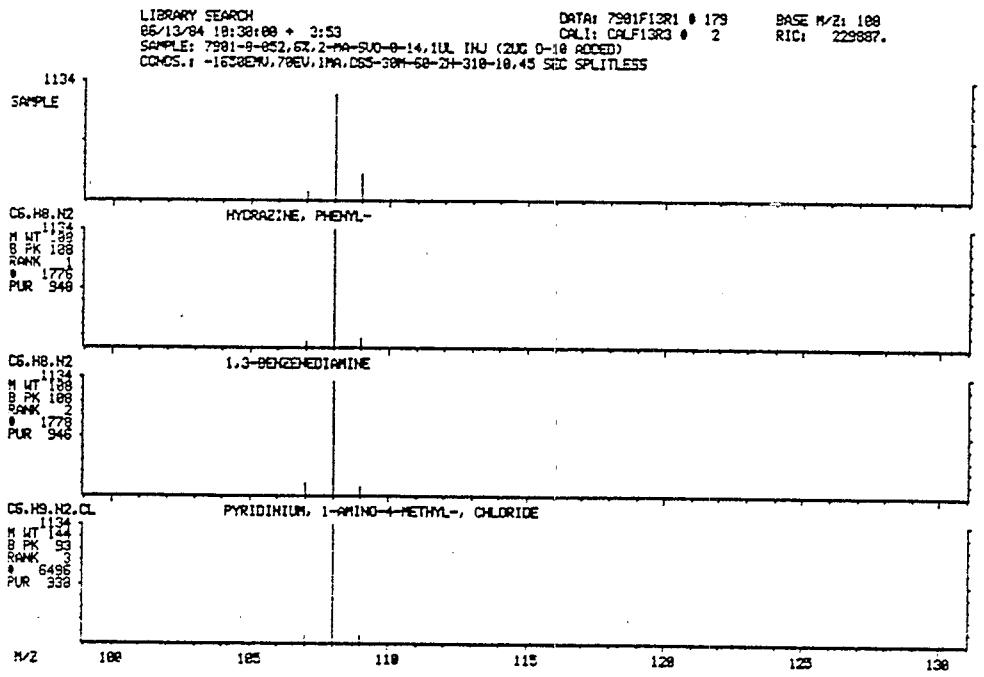

Figure 9. Library search results of an unknown peak with inadequate fragmentation for reliable identification. The upper plot in the lower figure is the mass spectrum of the unknown peak. Note that only four masses are present in the unknown spectrum. Poor fragmentation often results in multiple candidate spectra, as shown in the upper portion of the figure.

for semivolatiles) to compress the GC profile as much as possible. Unfortunately, this caused a number of unknown peaks to overlap and coelute.

The Incos data system contains enhancement software which attempts to deconvolute mixed spectra, but its success is dependent on the degree of overlap of the various GC peaks. As the overlap becomes greater and the number of overlapping compounds increases, the enhancement routine becomes less successful in deconvoluting spectra. Peaks with complete or nearly complete overlap cannot be deconvoluted at all.

The ACORN procedure always used enhanced spectra when conducting searches of the seed and NBS libraries. Despite this precaution, however, a number of mass spectra were analyzed which upon closer examination were found to be mixtures of two or more compounds. There did not appear to be a solution to this problem using the available data. Different operating conditions could be employed to optimize the analysis for unknown compound identification purposes. These could include a slower GC temperature program rate, use of a longer capillary column, or use of a Megabore column for volatile analysis. Of course, these changes would require reanalysis of at least a limited number of samples.

4. Background Contribution

A number of samples in the semivolatile fraction exhibited a hump-shaped RIC profile, shown in Figure 10, which is common for samples of biological origin. The hump exhibits a rather uniform spectrum throughout its entire length, which is shown in Figure 11. The presence of this hump throughout a major portion of the RICs interfered with attempts to extract high quality spectra of peaks located on the humps. The effect of the hydrocarbon hump was least acute for samples in the 0-14 age group and progressively influenced data quality in the higher age group samples. Figure 6, which was presented earlier in this text, illustrates the difference in the intensity of the hydrocarbon hump in proceeding from the 0-14 age group to the 45+ age group.

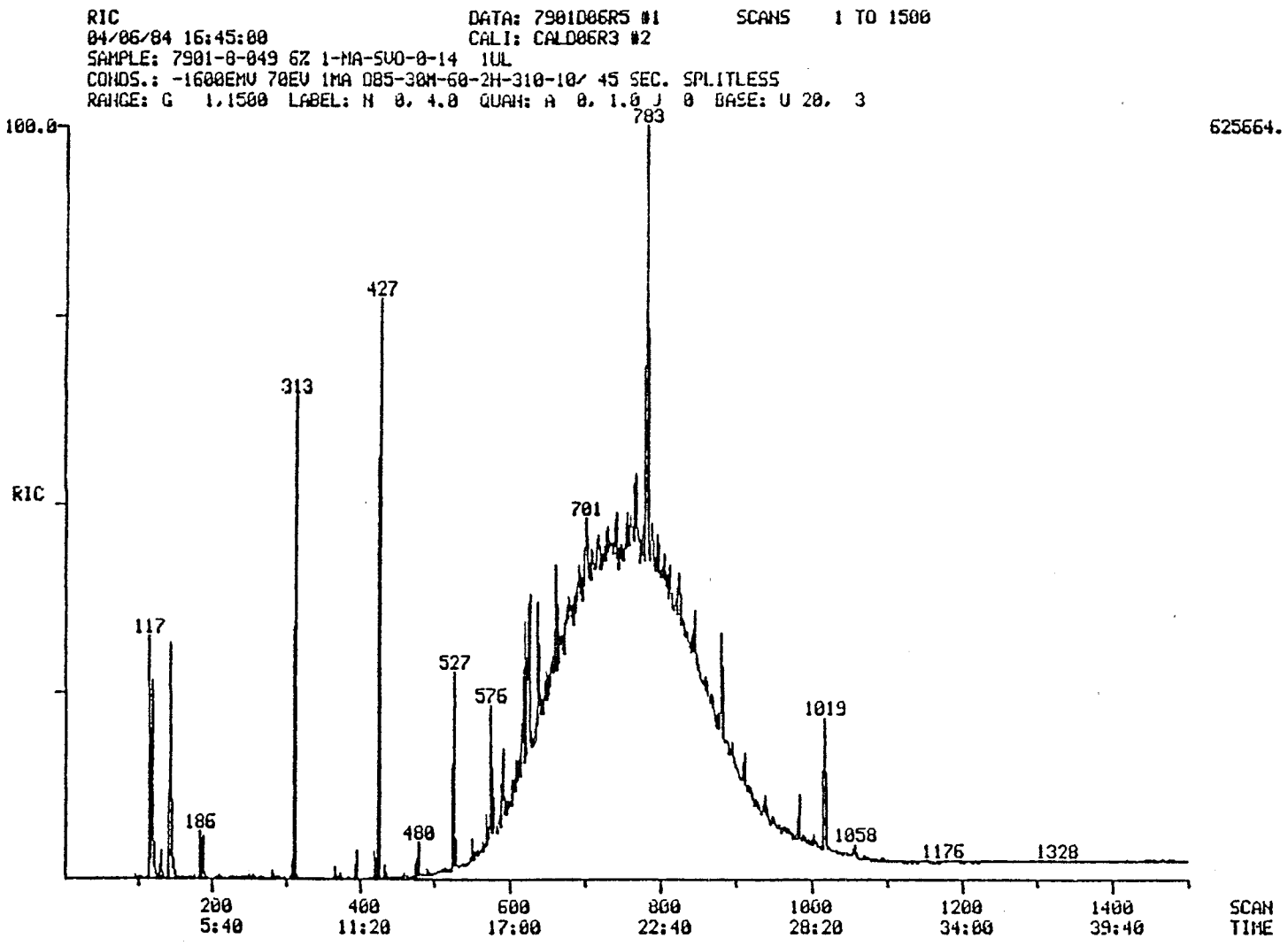

Figure 10. RIC chromatogram with hydrocarbon "hump."

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16. ABSTRACT

The National Human Adipose Tissue Survey (NHATS), administered by EPA/OTS, is an ongoing chemical monitoring network designed to detect levels and prevalences of toxic substances in the adipose tissue of the general U.S. population. Adipose specimens collected in fiscal year 1982 were analyzed as composites for volatile and semivolatile organic compounds via HRGC/MS as part of a previous effort. The data files were then processed using a method developed to automatically identify unknown HRGC/MS peaks. The method consisted of automatic identification of unknown spectra via comparisons to reference mass spectra, transfer of the results of the identification step to a microcomputer, compilation of the data into a spreadsheet program and generation of compound identification tables from the spreadsheet. Application of the method to the adipose data resulted in the identification of volatile compounds from 18 separate chemical classes and semivolatiles from 29 chemical classes. Compound classes included saturated and unsaturated hydrocarbons, aldehydes, ketones, steroids heterocyclic compounds, drugs, aliphatic and phthalate esters, phenols, halocarbons, and methyl-substituted organosiloxanes. Volume I (EPA-560/5-87-002A) describes the technical approach. Volume II (EPA-560/5-87-002B) provides supplemental data.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Grou
Adipose Computer program Mass spectrometry GC/MS Volatile Semivolatile Data transfer Characterization		

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