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Identification of SARA Compounds in Adipose Tissue

Final Report

By
Jon D. Onstot
John S. Stanley

For National Human Monitoring Program
Field Studies Branch (TS-798)
Exposure Evaluation Division
Office of Pesticides and Toxic Substances
401 M Street, SW
Washington, DC 20460

Attn: Ms. Janet Remmers, Work Assignment Manager
Dr. Joseph J. Breen, OTS Project Officer

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PREFACE

This report describes the methodology and results of a study to determine levels of selected volatile and semivolatile organic compounds selected for the Superfund Amendments and Reauthorization Act (SARA), Title III, Section 313 listing, in human adipose tissue.

This work was 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). The HRGC/MS data used in this study were originally generated under EPA Contract No. 68-02-3538, Work Assignment 8. In the original study, 46 composite samples were prepared from individual specimens obtained from the Environmental Protection Agency's National Human Adipose Tissue Survey (EPA NHATS fiscal year 1982 (FY82)) repository.

This report was prepared by Mr. Jon Onstot with assistance from Dr. John S. Stanley, MRI Work Assignment Leader. Additional work for this task was performed by Mr. Fred Forman and Ms. Audrey Zoog.

MIDWEST RESEARCH INSTITUTE

Paul C. Constant
Program Manager

Reviewed:

Jack Balsinger
Quality Assurance Coordinator

Approved:

John E. Going, Director
Chemical Sciences Department

TABLE OF CONTENTS

TABLE OF CONTENTS (continued)

LIST OF FIGURES

LIST OF TABLES

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. In 1984, the list of target compounds was expanded to include other volatile (VOA) and semivolatile organic (SMV) compounds as part of an effort to expand the use and capabilities of the NHATS program. This effort was undertaken to detect other potentially toxic compounds that might be entering the environment. This expanded target list was used in the broad scan analysis of adipose specimens collected during the FY82 (Stanley 1986). A follow-up study was directed at identifying high resolution gas chromatography/mass spectrometry (HRGC/MS) peaks in the FY82 data which had not been identified in the broad scan study (Onstot 1987). However, the latter study left open the possibility that additional compounds of interest might still be present in the data.

In the current study, an expanded list of target compounds was selected for analysis and was applied to the FY82 HRGC/MS data. Target compounds were selected from three existing listings: the Superfund Amendments and Reauthorization Act (SARA) Title III, Section 313 toxic chemical listing (*Fed. Reg.* 53:30); the SARA Section 110 listing (*Fed. Reg.* 52:74); and a listing of priority compounds which were tentatively identified in a previous study of the same data (Onstot 1987a, Onstot 1987b, Price 1987), hereafter referred to as the Existing Chemicals Assessment Division (ECAD) Listing. From these listings, 61 volatile and 120 semivolatile target compounds were selected and searched in the FY82 data. Application of target compound analysis (TCA) to 46 composited adipose tissue samples collected during FY82 resulted in the identification of 13 volatile and 19 semivolatile compounds. Frequency-of-occurrence data was compiled with respect to three age groups, four census regions and nine census divisions. The compounds were identified from three sample fractions: a volatile fraction and two semivolatile fractions produced from a cleanup step using 6% and 15/50% diethyl ether/hexane column chromatography fractions, respectively. A list of compounds identified in each of the sample fractions and frequencies of occurrence is shown below.

Volatile Compounds

No.	Compound	Frequency	313	110	ECAD
1.	2-Amylfuran	46			x
2.	Bromoheptane	4			x
3.	Bromopentane	3			x
4.	Butyraldehyde	45	x		
5.	Ethyl isovalerate	44	x		
6.	1-Iodopentane	35			x
7.	Isobutyraldehyde	43	x		
8.	Limonene	46			x
9.	Nonene	46			x
10.	3-Octen-2-one	45			x
11.	Pentyl alcohol	38			x
12.	Pentyl cyclohexane	10			x
13.	Trichloroethylene	20	x	x	

6% Florisil Fraction Semivolatile Compounds

No.	Compound	Frequency	313	110	ECAD
1.	Anthracene	1		x	
2.	Biphenyl	9	x		
3.	Cymene	41			x
4.	Dibenzofuran	3	x		
5.	Limonene	41			x
6.	Diphenyl ether	40			
7.	Safrole	4	x		
8.	1,2,4-Trimethylbenzene	42		x	
9.	2,6-Xylidene	11	x		

15/50% Florisil Fraction Semivolatile Compounds

No.	Compound	Frequency	313	110	ECAD
1.	Bis(2-ethylhexyl)adipate	8	x		
2.	Butyl glycol butyl phthalate	8			x
3.	Carbaryl	1	x		
4.	*o*-Cresol	38	x	x	
5.	*m,p*-Cresol	43	x		
6.	Di-(2-ethylhexyl) phthalate (DEHP)	42	x	x	
7.	2,4-Diaminotoluene	20	x		
8.	2-Ethoxy benzaldehyde	6			x
9.	4-Pentyl benzaldehyde	9			x
10.	2-Phenyl phenol	22	x		x

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 selected toxic compounds. The objective of the NHATS program is to detect the level and prevalences of these 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

In 1984, EPA/OTS recognized the need to provide a more comprehensive assessment of the toxic substances that accumulate in adipose tissue than was being provided at that time. An aggressive strategy to assess TSCA-related substances that persist in the adipose tissue of the general U.S. population was therefore 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 PCB's 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 a target list of volatile and semivolatile organic compounds by high resolution gas chromatography/mass spectrometry (HRGC/MS). This analysis approach is hereafter referred to as broad scan analysis.

B. Characterization of Unidentified Peaks

Although broad scan analysis provided EPA/OTS with an expanded list of potentially toxic compounds in adipose tissue, a much larger number of peaks were observed in the HRGC/MS reconstructed ion chromatograms (RIC) that were still not identified. A procedure was developed to automatically characterize these unidentified peaks (Onstot 1986a, Onstot 1986b) based on a forward library search approach. In this approach, an unknown mass spectrum is compared to a library of reference mass spectra, as opposed to a reverse search approach in which a single reference mass spectrum corresponding to a target compound is compared to the spectra in a GC/MS file.

Application of the automated peak identification procedure resulted in the tentative identification of 121 compounds in the VOA samples, 81 compounds in the 6% Florisil SMV, and 96 compounds in the 15/50% Florisil SMV samples. However, a significant number of peaks were still unable to be identified by the automated procedure, with 99 spectra from the volatile, 258 spectra from the 6% Florisil and 343 spectra from the 15/50% Florisil SMV fractions remaining unidentified at the end of that study. A number of reasons were cited to account for the inability of the procedure to identify these unknown peaks, which included a mass scanning range that was not suitable for the identification of unknown spectra, candidate mass spectra which were obviously not represented in the reference mass spectral library, and difficulties encountered in extracting high quality spectra from a complex sample matrix such as adipose. In addition, the peak selection process focused primarily on peaks which were visibly discernible above the total ion current baseline. As a result, the unidentified peaks study left open the possibility that additional compounds of interest might still be present in the data.

C. Work Assignment Objectives

A new approach for the identification of potentially significant compounds in the FY82 data was formulated which would be less susceptible to the problems encountered in the unidentified peaks study. The new approach consisted of a return to the analysis of a specific list of target analytes, as opposed to the forward library search approach used in the unidentified peaks study. Although target compound analysis (TCA), based on the reverse search approach, is more restrictive in the sense that identification is limited to only those compounds which have been preselected for study, such an approach provides a greater degree of selectivity and sensitivity than the forward library search.

Three compound listings were selected as sources for environmentally significant target compounds: the Superfund Amendments and Reauthorization Act (SARA) Title III, Section 313 toxic chemical listing; the SARA Section 110 listing; and a listing of 16 priority compounds which were tentatively identified in the unidentified peaks study and targeted by the Existing Chemicals Assessment Division (ECAD) of EPA as chemicals of interest. The latter listing was included in order to provide a check for those compounds which were identified in the original unidentified peaks study and which were deemed at that time to be environmentally significant.

The objectives for this task were to (1) evaluate the compounds in the above listings and determine whether they might be applicable as target compounds for the FY82 dataset; (2) categorize each candidate compound chosen from the listings according to the fraction (VOA or SMV) in which they would be expected to be observed, i.e., estimate their volatility; and (3) perform TCA on the set of FY82 composite samples.

D. Significance

The significance of this study is twofold. First, the use of the SARA listings for the selection of target compounds provides an opportunity for EPA to correlate information gathered from other studies using these lists with the information collected from the NHATS data. For example, the Section 110 listing, which is a prioritized list of compounds chosen from the 717 hazardous substances currently identified under Section 102 of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), represent compounds which have been determined to pose a potential human health risk and which have been identified at National Priorities List hazardous waste sites. Correlation of these human risk compounds with NHATS data would allow EPA to more accurately assess the danger of these compounds to the human population from environmental sources.

Secondly, compounds identified in this study may be selected for inclusion in the broad scan analysis of future NHATS samples. This would provide EPA with long-term bioaccumulation information which could be tracked for possible long-term trends, which could in turn be correlated to environmental levels determined from other studies as described above. The correlation of trends between levels of environmental pollutants and human bioaccumulation levels has been already been demonstrated through NHATS for several compounds including polychlorinated biphenyls (PCBs), hexachlorobenzene (HCB) and the DDT family.

E. Organization of This Report

Following this introductory section, Section II presents recommendations for pursuing future activities related to this study. Section III presents the experimental procedure and describes the process of selecting target compounds, developing the necessary criterion for supporting qualitative identification, and conducting the target compound analysis. The results of this experimental effort are presented in Section IV and a discussion of results and other findings is provided in Section V. Appendices A through C present amounts for the identified compounds compared to their respective internal standard response. Appendices D through F present the data in additional detail based on comparisons of identified compounds within census divisions and regions. Appendix G shows a representative mass spectral comparison of each identified compound to the reference library.

II. RECOMMENDATIONS

Recommendations for further activities in the area of TCA analysis of NHATS samples may be divided into four major areas, described below.

A. Analysis of Other NHATS FY Datafiles

One of the results of the current study was the construction of a mass spectral database for the quantitation of environmentally significant target compounds. Application of this quantitation library to subsequent NHATS samples would involve much less effort than was required in this study since the target compound selection and the library construction steps would not need to be repeated.

B. Recovery Efficiency Studies

In contrast to the broad scan study, no recovery efficiency studies were performed to determine to what extent the target compounds could be recovered by the extraction method used. Knowledge of extraction efficiencies would be useful in two regards. First, some compounds would almost certainly be found to be unrecoverable from adipose by the extraction method used on the FY82 data and could be eliminated from further consideration as target compounds in future studies. Secondly, recovery efficiency data would allow more precise estimates of concentration levels for compounds identified in adipose to be made.

C. Analysis of Future NHATS Samples

It is recommended that the compounds identified in this study be included in any future target compound analyses for the NHATS project. In this way, information regarding the incidence of occurrence in human adipose for the compounds identified in this study will be accumulated in the same way as for the compounds currently included in the Broad Scan target analyte listing.

III. EXPERIMENTAL PROCEDURE

The experimental procedure used in this study was comprised of three major steps. The first step involved the selection of a list of target compounds from the SARA and ECAD compound listings. In the second step, a table of GC retention indices was compiled for the selected target compounds. Retention values were either derived from experimental data or were predicted using a regression plot of boiling points vs retention indices of compounds with known retention. The third step involved the setup of the target compound analysis (TCA) search libraries and subsequent TCA analysis of the FY82 data. These three steps are described in detail in the following sections.

A. Selection of Target Compounds

As stated in the introduction, the list of target compounds used in this study were chosen from three primary sources: the Superfund Amendments and Reauthorization Act (SARA) Title III, Section 313 toxic chemical listing of 308 chemical substances and 20 chemical categories; the SARA Section 110 listing of 108 hazardous substances most commonly found at facilities on the CERCLA National Priorities List; and a listing of 16 priority compounds which were tentatively identified in the original unidentified peaks study (Onstot, 1986a) that have been targeted by ECAD as chemicals of interest.

One compound, 1-iodopentane, was tentatively identified in a volatile composite after completion of the original unidentified peaks study and thus was not included in that report. This compound was included in the volatile target analyte list in order to determine its frequency of occurrence in the other volatile composites. One compound, diphenyl ether, is listed in this report as a target compound even though it is not a member of the SARA listings. However, as a result of the GC/MS analysis of authentic standards for this study, the compound originally thought to be 2-phenyl phenol in the 6% fraction composites was actually identified as diphenyl ether. Thus, for reporting purposes, diphenyl ether is listed as a target analyte so that it may be included in the tables of identified compounds.

A number of compounds from the above listings were found to be common to more than one list. A cross-reference was compiled which lists each unique compound vs the source listings, as well as the list of original broad scan target analytes. The cross-reference listing is shown in Table 1, with compounds arranged in alphabetical order. Three-hundred and forty-nine unique compounds were identified from a combined total of 432 entries in the 313, 110, and ECAD listings, with 83 compounds found to be represented in more than one listing. In some instances, compounds found in more than one listing were assigned different names. Inconsistencies in nomenclature were resolved by comparison of CAS registry numbers. In addition to the individual compounds listed in the Section 313 listing, 20 chemical categories are also listed. Most of these classes are comprised of metallic compounds and complexes such as antimony, arsenic, barium, cadmium, copper and lead, and are not amenable to GC/MS analysis. Three chemical categories composed of organic compounds were listed: chlorophenols, glycol ethers, and polybrominated biphenyls (PBBs). Chlorophenols and PBBs were included as analytes in the broad scan survey. The glycol ethers were not considered for this study.

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
1	Acetaldehyde	75-07-0	X			
2	Acetamide	60-35-5	X			
3	Acetone	67-64-1	X			
4	Acetonitrile	75-05-8	X			
5	2-Acetylaminofluorene	53-96-3	X			
6	Acrolein	107-02-8	X	X		
7	Acrylamide	79-06-1	X			
8	Acrylic Acid	79-10-7	X			
9	Acrylonitrile	107-13-1	X	X		
10	Aldrin	309-00-2	X	X	X	
11	Allyl Chloride	107-05-1	X			
12	Aluminum (fume or dust)	7429-90-5	X			
13	Aluminum Oxide	1344-28-1	X			
14	1-Amino-2-methylanthraquinone	82-28-0	X			
15	2-Aminoanthraquinone	117-79-3	X			
16	4-Aminoazobenzene	60-09-3	X			
17	4-Aminobiphenyl	92-67-1	X			
18	Ammonia	7664-41-7	X	X		
19	Ammonium nitrate (solution)	6484-52-2	X			
20	Ammonium sulfate (solution)	7783-20-2	X			
21	2-Amyl furan	3777-69-3				X
22	Aniline	62-53-3	X	X		
23	p-Anisidine	104-94-9	X			
24	o-Anisidine	90-04-0	X			
25	o-Anisidine hydrochloride	134-29-2	X			
26	Anthracene	120-12-7	X			
27	Antimony	7440-36-0	X			
28	Arsenic	7440-38-2	X	X		
29	Asbestos (friable)	1332-21-4	X			
30	Barium	7440-39-3	X			
31	Benzal chloride	98-87-3	X			
32	Benzamide	55-21-0	X			
33	Benzene	71-43-2	X	X	X	
34	Benzidine	92-87-5	X	X		
35	Benzo(a)anthracene	56-55-3		X		
36	Benzo(a)pyrene	50-32-8		X		
37	Benzo(b)fluoranthene	205-99-2		X		
38	Benzoic acid	65-85-0		X		
39	Benzoic trichloride ([Trichloromethyl]benzene)	98-07-7	X			
40	Benzoyl chloride	98-88-4	X			
41	Benzoyl peroxide	94-36-0	X			
42	Benzyl chloride	100-44-7	X			
43	Beryllium	7440-41-7	X	X		
44	∂-BHC (c)	319-86-8		X	X	
45	a-BHC (c)	319-84-6		X	X	
46	ß-BHC (c)	319-85-7		X	X	
47	Lindane {g-BHC} (c)	58-89-9	X	X		
48	Biphenyl	92-52-4	X			

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
49	Bis(2-chloro-1-methylethyl)ether	108-60-1	X			
50	Bis(2-chloroethyl)ether	111-44-4	X	X		
51	Bis(2-ethylhexyl)adipate	103-23-1	X			
52	Bis(chloromethyl)ether	542-88-1	X	X		
53	Bromoform	75-25-2	X	X	X	
54	Bromoheptane	629-04-9				X
55	Bromomethane	74-83-9	X	X		
56	Bromopentane	110-53-2				X
57	1,3-Butadiene	106-99-0	X			
58	Butyl Acrylate	141-32-2	X			
59	tert-Butyl alcohol	75-65-0	X			
60	n-Butyl Alcohol	71-36-3	X			
61	sec-Butyl alcohol	78-92-2	X			
62	Butyl benzyl phthalate	85-68-7	X		X	
63	Butyl glycol butyl phthalate	85-70-1				X
64	1,2-Butylene oxide	106-88-7	X			
65	Butyraldehyde	123-72-8	X			
66	C.I. Acid Blue 9, diammonium salt	2650-18-2	X			
67	C.I. Acid Blue 9, disodium salt	3844-45-9	X			
68	C.I. Acid Green 3	4680-78-8	X			
69	C.I. Basic Green 4	569-64-2	X			
70	C.I. Basic Red 1	989-38-8	X			
71	C.I. Direct Black 38	1937-37-7	X			
72	C.I. Direct Blue 6	2602-46-2	X			
73	C.I. Direct Brown 95	16071-86-6	X			
74	C.I. Disperse Yellow 3	2832-40-8	X			
75	C.I. Food Red 15	81-88-9	X			
76	C.I. Food Red 5	3761-53-3	X			
77	C.I. Solvent Orange 7	3118-97-6	X			
78	C.I. Solvent Yellow 14	842-07-9	X			
79	C.I. Solvent Yellow 3	97-56-3	X			
80	C.I. Solvent Yellow 34	492-80-8	X			
81	C.I. Vat Yellow 4	128-66-5	X			
82	Cadmium	7440-43-9	X	X		
83	Calcium cyanamide	156-62-7	X			
84	Captan	133-06-2	X			
85	Carbaryl	63-25-2	X			
86	Carbon disulfide	75-15-0	X	X		
87	Carbon tetrachloride	56-23-5	X	X		
88	Carbonyl sulfide	463-58-1	X			
89	Catechol	120-80-9	X			
90	Chloramben	133-90-4	X			
91	Chlordane	57-74-9	X	X	X	
92	Chlorine	7782-50-2	X			
93	Chlorine dioxide	10049-04-4	X			
94	p-Chloro-m-cresol	59-50-7		X		
95	Chloroacetic acid	79-11-8	X			
96	2-Chloroacetophenone (Tear gas)	532-27-4	X			

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
97	Chlorobenzene	108-90-7	X	X	X	
98	Chlorobenzilate	510-15-6	X			
99	Chlorodibromomethane	124-48-1		X	X	
100	Chloroethane	75-00-3	X	X		
101	Chloroform	67-66-3	X	X	X	
102	Chloromethane	74-87-3	X	X		
103	Chloromethyl methyl ether	107-30-2	X			
104	Chloroprene	126-99-8	X			
105	Chlorothalonil	1897-45-6	X			
106	Chromium	7440-47-3	X	X		
107	Chrysene	218-01-9		X	X	
108	Cobalt	7440-48-4	X			
109	Copper	7440-50-8	X	X		
110	p-Cresidine	120-71-8	X			
111	o-Cresol (o-methylphenol)	95-48-7	X	X		
112	p-Cresol (p-methylphenol)	106-44-5	X			
113	m-Cresol (m-methylphenol)	108-39-4	X			
114	Cresols, Mixed (d)	1319-77-3	X			
115	Cumene (isopropylbenzene)	98-82-8	X			
116	Cumene hydroperoxide	80-15-9	X			
117	Cupferron	135-20-6	X			
118	Cyanide (e)	57-12-5		X		
119	Cyclohexane	110-82-7	X			
120	Cymene (isopropyltoluene)	99-87-6				X
121	2,4-D	94-75-7	X			
122	4,4'-DDD (f)	72-54-8		X	X	
123	4,4'-DDE (f)	72-55-9		X	X	
124	4,4'-DDT (f)	50-29-3		X	X	
125	Decabromodiphenyl oxide	1163-19-5	X			
126	Di-(2-ethylhexyl)phthalate {Bis(2-ethylhexyl)phthalate}	117-81-7	X	X		
127	Di-n-octyl phthalate	117-84-0	X		X	
128	Diallate	2303-16-4	X			
129	2,4-Diaminoanisole	615-05-4	X			
130	2,4-Diaminoanisole sulfate	39156-41-7	X			
131	4,4'-Diaminodiphenyl ether	101-80-4	X			
132	2,4-Diaminotoluene	95-80-7	X			
133	Diaminotoluene (mixed isomers)	25376-45-8	X			
134	Diazomethane	334-88-3	X			
135	Dibenz(a,h)anthracene	53-70-3		X		
136	Dibenzofuran	132-64-9	X			
137	1,2-Dibromo-3-chloropropane	96-12-8	X			
138	1,2-Dibromoethane (Ethylene bromide)	106-93-4	X			
139	Dibutyl phthalate {Di-n-butyl phthalate}	84-74-2	X	X	X	
140	1,2-Dichlorobenzene	95-50-1	X	X	X	
141	1,4-Dichlorobenzene	106-46-7	X	X	X	
142	1,3-Dichlorobenzene	541-73-1	X	X	X	
143	Dichlorobenzenes (mixed isomers)	25321-22-6	X			
144	3,3'-Dichlorobenzidine	91-94-1	X	X		

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
145	Dichlorobromomethane {Bromodichloromethane}	75-27-4	X	X	X	
146	Dichlorodifluoromethane (Freon 12)	75-71-8		X		
147	1,2-Dichloroethane	107-06-2	X	X		
148	1,1-Dichloroethane	75-34-3		X		
149	1,2-Dichloroethylene {1,2-Dichloroethene}	540-59-0	X	X		
150	Dichloromethane {Methylene Chloride}	75-09-2	X	X	X	
151	2,4-Dichlorophenol	120-83-2	X	X	X	
152	1,2-Dichloropropane	78-87-5	X	X		
153	1,3-Dichloropropylene	542-75-6	X			
154	Dichlorvos	62-73-7	X			
155	Dicofol	115-32-2	X			
156	Dieldrin	60-57-1		X	X	
157	Diepoxybutane	1464-53-5	X			
158	Diethanolamine	111-42-2	X			
159	Diethyl phthalate	84-66-2	X	X	X	
160	Diethyl sulfate	64-67-5	X			
161	3,3'-Dimethoxybenzidine	119-90-4	X			
162	1,1-Dimethyl hydrazine	57-14-7	X			
163	2,4-Dimethyl phenol	105-67-9	X	X		
164	Dimethyl phthalate	131-11-3	X	X		
165	Dimethyl sulfate	77-78-1	X			
166	4-Dimethylaminoazobenzene	60-11-7	X			
167	3,3'-Dimethylbenzidine (o-Tolidine)	119-93-7	X			
168	Dimethylcarbamyl chloride	79-44-7	X			
169	4,6-Dinitro-o-cresol {4,6-Dinitro-2-methylphenol}	534-52-1	X	X		
170	2,4-Dinitrophenol	51-28-5	X	X		
171	2,4-Dinitrotoluene	121-14-2	X	X		
172	2,6-Dinitrotoluene	606-20-2	X	X		
173	1,4-Dioxane	123-91-1	X	X		
174	p-Dioxin	1745-01-6		X		
175	1,2-Diphenyl hydrazine	122-66-7	X	X		
176	Endrin (g)	72-20-8		X	X	
177	Endrin Aldehyde (g)	7421-93-4		X	X	
178	Epichlorohydrin	106-89-8	X			
179	2-Ethoxy benzaldehyde	613-69-4				X
180	2-Ethoxyethanol	110-80-5	X			
181	Ethyl acrylate	140-88-5	X			
182	Ethyl chloroformate	541-41-3	X			
183	Ethyl isovalerate	108-64-5				X
184	Ethylbenzene	100-41-4	X	X	X	
185	Ethylene	74-85-1	X			
186	Ethylene glycol	107-21-1	X			
187	Ethylene oxide {Oxirane}	75-21-8	X	X		
188	Ethylene thiurea	96-45-7	X			
189	Ethyleneimine (Aziridine)	151-56-4	X			
190	Fluometuron	2164-17-2	X			
191	Fluoranthene	206-44-0		X	X	
192	Fluorotrichloromethane (Freon 11)	75-69-4		X		

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
193	Formaldehyde	50-00-0	X			
194	Freon 113	76-13-1	X			
195	Heptachlor (h)	76-44-8	X	X	X	
196	Heptachlor Epoxide (h)	1024-57-3		X	X	
197	Hexachloro-1,3-butadiene	87-68-3	X	X		
198	Hexachlorobenzene	118-74-1	X	X	X	
199	Hexachlorocyclopentadiene	77-47-4	X			
200	Hexachloroethane	67-72-1	X	X		
201	Hexachloronaphthalene	1335-87-1	X			
202	Hexamethylphosphoramide	680-31-9	X			
203	1-Hexene	592-41-6				X
204	Hydrazine	302-01-2	X			
205	Hydrazine sulfate	10034-93-2	X			
206	Hydrochloric acid	7647-01-0	X			
207	Hydrogen cyanide	74-90-8	X			
208	Hydrogen fluoride	7664-39-3	X			
209	Hydroquinone	123-31-9	X			
210	Indeno(1,2,3-cd)pyrene	193-39-5		X		
211	Isobutyraldehyde	78-84-2	X			
212	Isophorone	78-59-1		X		-
213	Isopropyl alcohol	67-63-0	X			
214	4,4'-Isopropylidenediphenol	80-05-7	X			
215	Lead	7439-92-1	X	X		
216	Limonene	138-86-3				X
217	Maleic anhydride	108-31-6	X			
218	Maneb	12427-38-2	X			
219	Manganese	7439-96-5	X			
220	Melamine	108-78-1	X			
221	Mercury	7439-97-6	X	X		
222	Methanol	67-56-1	X			
223	Methoxychlor	72-43-5	X			
224	2-Methoxyethanol	109-86-4	X			
225	Methyl acrylate	96-33-3	X			
226	Methyl ethyl ketone {2-Butanone}	78-93-3	X	X		
227	Methyl hydrazine	60-34-4	X			
228	Methyl iodide	74-88-4	X			
229	Methyl isobutyl ketone {4-Methyl-2-pentanone}	108-10-1	X	X		
230	Methyl isocyanate	624-83-9	X			
231	Methyl methacrylate	80-62-6	X			
232	Methyl tert-butyl ether	1634-04-4	X			
233	Methylene bromide	74-95-3	X			
234	4,4'-Methylenebis(2-chloroaniline)	101-14-4	X			
235	4,4'-Methylenebis(N,N-dimethyl)benzenamine	101-61-1	X			
236	Methylenebis(phenylisocyanate) (MBI)	101-68-8	X			
237	4,4'-Methylenedianiline	101-77-9	X			
238	Michler's ketone	90-94-8	X			
239	Molybdenum trioxide	1313-27-5	X			
240	Mustard gas (1,1'-Thiobis[2-chloro-]ethane)	505-60-2	X			

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
241	N,N-Dimethylaniline	121-69-7	X			
242	N-Nitroso-N-ethylurea	759-73-9	X			
243	N-Nitroso-N-methylurea	684-93-5	X			
244	N-Nitrosodi-n-butylamine	924-16-3	X			
245	N-Nitrosodi-n-propylamine	621-64-7	X	X		
246	N-Nitrosodiethylamine	55-18-5	X			
247	N-Nitrosodimethylamine	62-75-9	X	X		
248	N-Nitrosodiphenylamine	86-30-6	X	X		
249	N-Nitrosomethylvinylamine	4549-40-0	X			
250	N-Nitrosomorpholine	59-89-2	X			
251	N-Nitrosonornicotine	16543-55-8	X			
252	N-Nitrosopiperidine	100-75-4	X			
253	Naphthalene	91-20-3	X	X	X	X
254	ß-Naphthylamine	91-59-8	X			
255	a-Naphthylamine	134-32-7	X			
256	Nickel	7440-02-0	X	X		
257	Nitric acid	7697-37-2	X			
258	Nitrilotriacetic acid	139-13-9	X			
259	5-Nitro-o-anisidine	99-59-2	X			
260	Nitrobenzene	98-95-3	X	X		
261	4-Nitrobiphenyl	92-93-3	X			
262	Nitrofen	1836-75-5	X			
263	Nitrogen mustard	51-75-2	X			
264	Nitroglycerin	55-63-0	X			
265	2-Nitrophenol	88-75-5	X			
266	4-Nitrophenol	100-02-7	X			
267	2-Nitropropane	79-46-9	X			
268	p-Nitrosodiphenylamine	156-10-5	X			
269	Nonene	124-11-8				X
270	Octachloronaphthalene	2234-13-1	X			
271	3-Octen-2-one	1669-44-9				X
272	Osmium tetroxide	20816-12-0	X			
273	Parathion	56-38-2	X			
274	Pentachlorophenol (PCP)	87-86-5	X	X	X	
275	1-Pentyl Alcohol	71-41-0				X
276	4-Pentyl benzaldehyde	6853-57-2				X
277	Pentyl cyclohexane	4292-92-6				X
278	Peracetic acid	79-21-0	X			
279	Phenanthrene	85-01-8		X	X	
280	Phenol	108-95-2	X	X		
281	2-Phenyl phenol (o-Phenol phenol)	90-43-7	X			X
282	p-Phenylenediamine	106-50-3	X			
283	Phosgene	75-44-5	X			
284	Phosphoric acid	7664-38-2	X			
285	Phosphorus (yellow or white)	7723-14-0	X			
286	Phthalic anhydride	85-44-9	X			
287	Picric acid	88-89-1	X			
288	Polychlorinated biphenyls (PCB'S)	1336-36-3	X	X	X	

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
289	Propane sulfone	1120-71-4	X			
290	ß-Propiolactone	57-57-8	X			
291	Propionaldehyde	123-38-6	X			
292	Propoxur	114-26-1	X			
293	Propylene	115-07-1	X			
294	Propylene oxide	75-56-9	X			
295	Propyleneimine	75-55-8	X			
296	Pyridine	110-86-1	X			
297	Quinoline	91-22-5	X			
298	Quinone	106-51-4	X			
299	Quintozene (Pentachloronitrobenzene)	82-68-8	X			
300	Saccharin	81-07-2	X			
301	Safrole	94-59-7	X			
302	Selenium	7782-49-2	X	X		
303	Silver	7440-22-4	X	X		
304	Sodium hydroxide (solution)	1310-73-2	X			
305	Sodium sulfate (solution)	7757-82-6	X			
306	Styrene	100-42-5	X		X	
307	Styrene oxide	96-09-3	X			
308	Sulfuric acid	7664-93-9	X			
309	Terephthalic acid	100-21-0	X			
310	1,1,2,2-Tetrachloroethane	79-34-5	X	X	X	
311	Tetrachloroethylene {Tetrachloroethene}	127-18-4	X	X	X	
312	Tetrachlorvinphos	961-11-5	X			
313	Thallium	7440-28-0	X	X		
314	Thioacetamide	62-55-5	X			
315	4,4'-Thiodianiline	139-65-1	X			
316	Thiourea	62-56-6	X			
317	Thorium dioxide	1314-20-1	X			
318	Titanium dioxide	13463-67-7	X			
319	Titanium tetrachloride	7550-45-0	X			
320	Toluene	108-88-3	X	X	X	
321	Toluene-2,4-diisocyanate	584-84-9	X			
322	Toluene-2,6-diisocyanate	91-08-7	X			
323	o-Toluidine	95-53-4	X			
324	o-Toluidine hydrochloride	636-21-5	X			
325	Toxaphene	8001-35-2	X	X	X	
326	Triaziquinone	68-76-8	X			
327	Trichlorfon	52-68-6	X			
328	1,2,4-Trichlorobenzene	120-82-1	X	X	X	
329	1,1,1-Trichloroethane	71-55-6	X	X	X	
330	1,1,2-Trichloroethane	79-00-5	X	X	X	
331	Trichloroethylene {Trichloroethene}	79-01-6	X	X		
332	2,4,6-Trichlorophenol	88-06-2	X	X	X	
333	2,4,5-Trichlorophenol	95-95-4	X		X	
334	Trifluralin	1582-09-8	X			
335	1,2,4-Trimethylbenzene	95-63-6	X			
336	Tris(2,3-dibromopropyl) phosphate	126-72-7	X			

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD
337	Urethane (Ethyl carbamate)	51-79-6	X			
338	Vanadium (fume or dust)	7440-62-2	X			
339	Vinyl acetate	108-05-4	X			
340	Vinyl bromide	593-60-2	X			
341	Vinyl chloride	75-01-4	X	X		
342	Vinylidene chloride {1,1-Dichloroethene}	75-35-4	X	X		
343	o-Xylene	95-47-6	X		X	
344	p-Xylene	106-42-3	X		X	
345	m-Xylene	108-38-3	X		X	
346	Xylene (mixed isomers) (d)	1330-20-7	X	X		
347	2,6-Xylidine	87-62-7	X			
348	Zinc	7440-66-6	X	X		
349	Zineb	12122-67-7	X			
		Total	308	108	49	16

Section 313 Chemical Categories

No	Compound Name	313	110	BS	ECAD
1	Antimony Compounds	X			
2	Arsenic Compounds	X			
3	Barium Compounds	X			
4	Berylium Compounds	X			
5	Cadmium Compounds	X			
6	Chlorophenols (d)	X		X	
7	Chromium Compounds	X			
8	Cobalt Compounds	X			
9	Copper Compounds	X			
10	Cyanide Compounds	X			
11	Glycol Ethers	X			
12	Lead Compounds	X			
13	Manganese Compounds	X			
14	Mercury Compounds	X			
15	Nickel Compounds	X			
16	Polybrominated Biphenyls	X		X	
17	Selenium Compounds	X			
18	Silver Compounds	X			
19	Thallium Compounds	X			
20	Zinc Compounds	X			

Notes:

a. Alternate names are shown in parentheses; names used in the Section 110 listing are shown in braces

b. Listing headers are as follows:
313 - SARA Section 313 Compounds

Table 1 - Cross Reference of Compounds Considered for Target Compound Analysis

No	Compound Name (a)	C.A.S.#	Listing (b) 313	110	BS	ECAD

110 - SARA Section 110 Compounds
BS - FY82 Broad Scan Target Analytes
ECAD - Existing Chemicals Assessment Division/NHMP Workgroup Compounds

c. BHC's are classed as a single target substance in the Section 110 listing
d. Individual isomers are also listed; the mixed substance was not considered as a separate candidate in this study.
e. Cyanide is included in the Section 313 listing under the Chemical Categories grouping as "Cyanide Compounds".
f. DDD, DDE and DDT are classed as a single target substance in the Section 110 listing.
g. Endrin and endrin aldehyde are classed as a single target substance in the Section 110 listing.
h. Heptachlor and heptachlor epoxide are classed as a single target substance in the Section 110 listing.

A large number of compounds from the SARA listings, including those from chemical classes such as inorganic gases, metals, metal salts, and dyes were eliminated a priori because these compound classes are not chromatographable under conditions used to generate the FY82 data.

B. Compilation of Physical Data

Physical data, consisting of boiling point, melting point, empirical formula, molecular weight, vapor pressure and existing GC retention indices, when available, were compiled for the candidate compounds. This information was used to divide the candidate list into two sublists corresponding to the volatile and semivolatile sample fractions. Existing GC information was considered the most reliable source for predicting in which sample fraction a compound would be found, and was given priority over other physical data. Two resources for GC retention information, EPA Method 1624/1625 (Rev. C, 1986), and EPA Report "GC/MS Suitability Testing of RCRA Appendix VIII and Michigan List Analytes" (Lucas 1987), proved useful in dividing the candidate list into volatile and semivolatile (VOA and SMV, respectively) sublists. Both of these references employed sample preparation and analysis schemes similar to the NHATS analyses. Lucas also listed a number of compounds from the Appendix VIII/Michigan lists which were found to be unsuitable for GC/MS analysis, many of which were common to the SARA lists. Compounds reported as unamenable to GC/MS analysis in the Lucas report were eliminated from further consideration as target analytes in this study.

In the absence of existing GC retention or volatility information, prediction was based primarily on boiling point. A boiling point of 150°C was used as the lower limit in the selection of semivolatile compounds, while compounds having boiling points below that value were assigned to the volatile list. However, a considerable amount of overlap between the volatile and the semivolatile fraction was observed, when the boiling points of the ECAD compounds in the two fractions were compared with the last observed volatile ECAD compound, pentyl cyclohexane, having a boiling point of 202°C. Limonene, with a boiling point of 178°C, was observed in both the volatile and 6% SMV fractions in the unidentified peaks study. As stated previously, experimentally derived GC retention data were preferred over boiling point alone, and as a result pentyl cyclohexane was assigned to the VOA fraction and limonene was included in both the VOA and SMV fractions. However, regardless of whether existing volatility data or boiling point was used as the determining criterion, no compound was added to the SMV fraction with a boiling point less than 150°C, which corresponds to the boiling point range for C3 alkyl benzenes such as cumene and 1,2,4-trimethylbenzene.

C. Final Selection of Analytes

Two limitations of the FY82 data itself affected the final selection of compounds for the target list. The first limitation was that the FY82 semivolatile samples were analyzed using a lower mass limit of 100 amu. Thus, compounds with a molecular weight below 100 amu were not detected at the time of analysis. As a result, a lower molecular weight limit of 110 amu was employed to eliminate candidate compounds whose mass spectra would not produce a sufficient number of mass peaks above 100 amu for reliable spectral matching

to take place. Examples of such compounds are phenol (mol. wt. 94) and diepoxybutane (mol. wt. 86). However, one exception to the 110 amu limit was made for cresols, which exhibit a distinctive M/M-1 isotope pattern at 107 and 108 amu. This isotope pattern, along with known GC retention and boiling point information, was sufficient to provide a reasonable degree of confidence for tentative identification of the three cresol isomers.

The second limitation to the existing FY82 data was that the GC conditions used in the VOA analysis precluded the observation of compounds with boiling points lower than approximately 40°C. A few compounds from the SARA listings had boiling points below 40°C and were eliminated from further consideration. Examples of compounds with low boiling points are chloromethane (BP -98°C) and ethylene (BP -104°C).

It should be noted that no recovery efficiency studies were performed to determine whether the candidate compounds could actually be recovered from adipose by the procedures used to generate the FY82 data. As a result, no candidate compounds were eliminated from consideration solely on the basis of their expected recoverability or recovery efficiency. Although recovery information would have been useful in eliminating unrecoverable compounds from the final list of target analytes, the time required to generate such data would have been much greater than performing target compound analysis for the compounds themselves. However, by using this approach it also follows that a negative identification of a target analyte did not necessarily constitute a negative identification in the FY82 adipose itself but rather demonstrated that the compound was not observed in the FY82 HRGC/MS data itself. Further studies to determine recovery efficiencies for the target analytes would allow a more accurate assessment to be made regarding the applicability of certain compounds to this analysis.

D. Prediction of GC Retention Values

In order for the target compound analysis procedure to search a GC/MS run for an analyte, two pieces of information pertaining to the analyte must be available to the procedure: the compound's mass spectrum and its relative retention time, determined against an internal standard. Since experimentally determined GC retention data could not be found for all candidate target compounds, a scheme for predicting relative retention values was used. In this scheme, compounds with known relative retention time (RRT) values and boiling points were selected and a regression curve of RRT vs. boiling point was computed. Predicted RRT values were then obtained via interpolation for compounds with known boiling points. Sources of known RRT values included data from the broad scan and unidentified peaks studies, EPA Methods 1624/1625, and the Lucas study. Boiling points were located from a number of sources, including the *CRC Handbook of Chemistry and Physics*, the *Merck Index*, and others.

Since RRT values from several different sources were used to create the regression curves, some normalization of RRT values was required. In particular, the semivolatile RRT values from the Lucas report differed by approximately 22% from those reported in the Method 1624/1625 protocol and the original broad scan study. The Lucas RRT values were adjusted to reflect this difference prior to their application in the regression computations. There was relatively close agreement of RRT values between the various sources, due primarily to similar GC conditions as shown in Table 2. However, it was found that there was a higher correlation of regression when only in-house generated retention values derived from the broad scan analytes were used. Thus, only RRTs from the broad scan survey were used to predict RRTs for the candidate target compounds in this study. Although the number of broad scan analytes was considerably smaller than the total number of compounds with RRT values from other sources, the broad scan analytes provided a more accurate prediction of RRT because they more closely represented the actual GC conditions in effect at the time of analysis.

A commercially available statistical computer program (StatView 512+, BrainPower, Inc.) was used to generate the regression plots of boiling point versus measured RRT. The program then automatically computed the predicted RRT values for the remaining candidate compounds. The regression curves for VOA and SMV compounds are shown in Figures 1 and 2 and tabular listings of RRT values and boiling points for VOA and SMV compounds used in the regression computations are shown in Tables 3 and 4, respectively. A polynomial regression was used for the volatiles, which provided a better approximation for that data than the linear regression used for the semivolatiles.

For a small number of semivolatile candidate target compounds, neither retention data nor boiling points could be located. As a result, retention could not be predicted for these compounds by the above scheme. In these cases, an alternative searching scheme based on manual examination of mass chromatograms was employed, which is described in the TCA analysis description below. A listing of compounds which were manually determined is provided in Table 5.

Reference mass spectra for the selected target compounds were located in the NBS Library of Mass Spectra (Heller, Milne 1983) containing 42,222 compounds. Seven compounds were not represented in the NBS library and were eliminated from further consideration as target compounds.

At this point, all unsuitable compounds had been eliminated from the candidate target compound listing, with all remaining compounds comprising the final target compound list. The final lists of compounds selected for volatile and semivolatile TCA analysis is shown in Tables 6 and 7, respectively. Compounds eliminated from further consideration as target analytes for this study are listed in Table 8. This table includes all eliminated compounds, including broad scan analytes and compounds eliminated a priori. A brief justification for elimination is provided for each compound.

Table 2 - GC Parameters of GC/MS Systems Used for Predicting RRT

GC/MS System	GC Column	Carrier Gas	GC Program
Semivolatile Analysis			
Method 1624/1625	30 meter DB-5 fused silica cap. column 0.25 mm ID, .25 micron film thickness	He, ca. 30cm/sec.	5 min. at 30 C 8 C/min. to 280 C hold until end of run
Broad Scan Study	30 meter DB-5 fused silica cap. column 0.25 mm ID, .25 micron film thickness	He, ca. 30cm/sec.	2 min. at 60 C 10 C/min. to 310 C hold until end of run
Lucas	30 meter DB-5 fused silica cap. column 0.25 mm ID, .25 micron film thickness	He, ca. 30cm/sec.	4 min at 30 C 8 C/min. to 300 C until end of run
Volatile Analysis			
Method 1624/1625	2.4 meter 1% SP-1000 packed column 2mm ID	He, 30 ml/min.	6 min. at 40 C 8 C/min. to 240 C hold until end of run
Broad Scan Study	30 meter DB-5 fused silica cap. column 0.25 mm ID, .25 micron film thickness	He, ca. 30cm/sec.	5 min. at 30 C 6 C/min. to 125 C hold until end of run
Lucas	6 ft. x 2 mm ID glass packed column 1% SP1000 on Carbopack B 60/80	He, 30 ml/min.	3 min. at 45 C 8 C/min to 220 C hold until end of run

Table 3

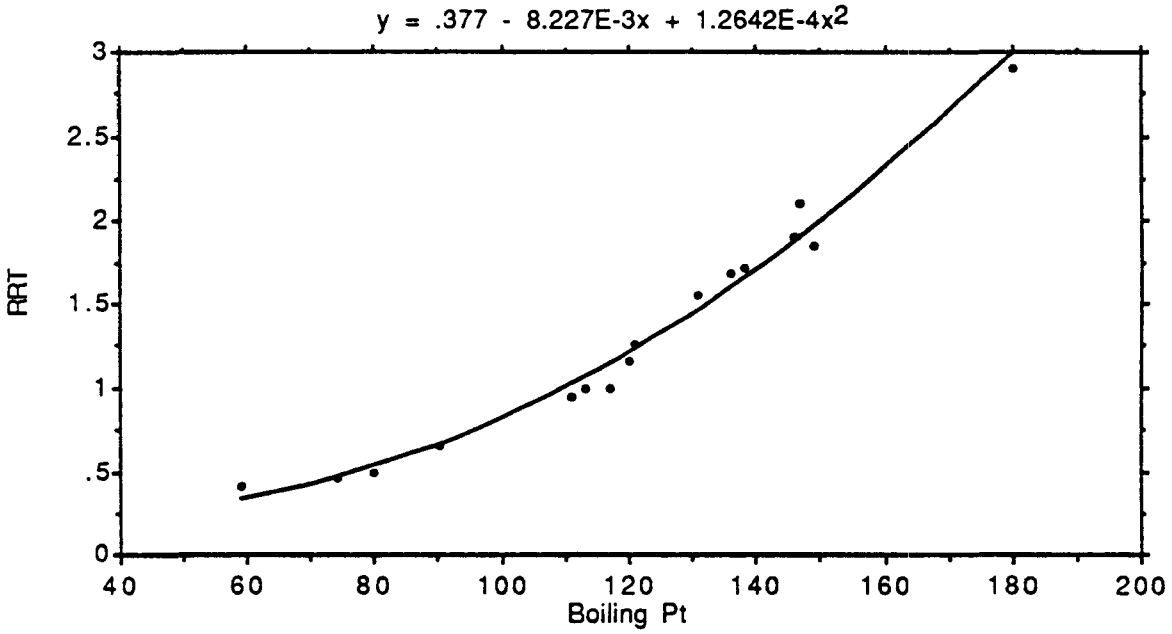
FY82 Broad Scan Target Analytes Used to Predict
Volatile RRT Values for SARA/ECAD Compounds

No.	Compound Name	Boiling Pt C (a)	RRT (b)
1	2-Bromo1-chloropropane	117	1.000
2	Chloroform	59	0.405
3	1,1,1-Trichloroethane	74	0.458
4	Benzene	80	0.498
5	Dichlorobromomethane	90	0.648
6	Toluene	111	0.947
7	1,1,2-Trichloroethane	113	0.996
8	Dibromochloromethane	120	1.162
9	Tetrachloroethylene	121	1.257
10	Chlorobenzene	131	1.555
11	Ethylbenzene	136	1.681
12	p-Xylene	138	1.715
13	Bromoform	149	1.852
14	Styrene	146	1.907
15	1,1,2,2-Tetrachloroethane	147	2.102
16	1,2-Dichlorobenzene	180	2.898

Notes:

a. Boiling points obtained from one or more of the following sources:
CRC Handbook of Chemistry and Physics 57th Edition
Merck Index 10th Edition 1983
Eastman Chemical Catalog 1988
Aldrich Chemical Catalog 1988-1989
EPA Method 1624/1625 Rev C
Chemical Hazardous Resource Information Service, DOT 1984
Int. Agency for Res. on Cancer, Monographs Vol. 1-42
Hazardous Substances Database, an online service of the
National Library of Medicine

b. Relative retention values derived from the FY82 Broad Scan Study (Stanley, 1986b)



Note: Plot based on RRT data shown in Table 3.

Figure 1. Regression plot of volatiles with known boiling point vs. RRT.

Table 4

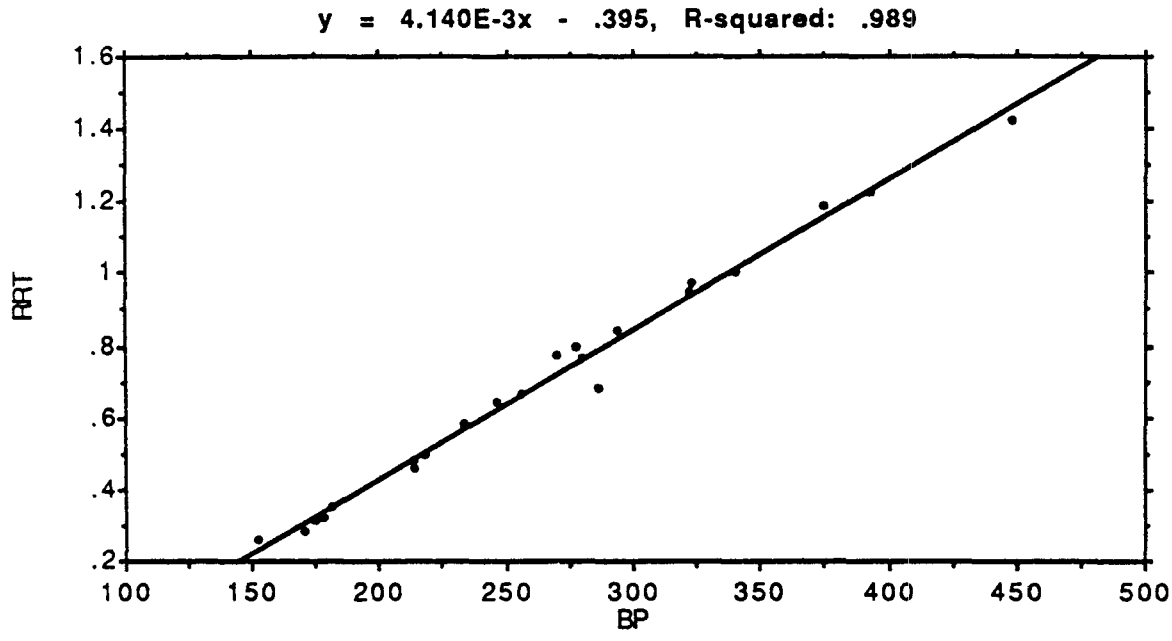
FY82 Broad Scan Target Analytes and Unidentified Peaks Compounds Used to Predict Semivolatile RRT Values for SARA/ECAD Analytes

No.	Compound Name	Boiling Pt C (a)	RRT	Source (b)
1	D10 Anthracene	340	1.000	UP
2	Cumene	152	0.263	UP
3	Trimethylbenzene	170	0.287	UP
4	Cymene	175	0.315	UP
5	Limonene	178	0.319	UP
6	Xylidene	213	0.459	UP
7	Safrole	233	0.582	UP
8	Biphenyl	256	0.669	UP
9	o-Phenyl Phenol	286	0.683	UP
10	1,2-Dichlorobenzene	181	0.353	BS
11	1,2,4-Trichlorobenzene	214	0.486	BS
12	Naphthalene	218	0.495	BS
13	2,4,6-Trichlorophenol	246	0.646	BS
14	Acenaphthene	279	0.765	BS
15	Acenaphthylene	270	0.775	BS
16	Pentachlorobenzene	277	0.793	BS
17	Fluorene	293	0.845	BS
18	Hexachlorobenzene	322	0.946	BS
19	ß-BHC	323	0.976	BS
20	Fluoranthene	375	1.189	BS
21	Pyrene	393	1.224	BS
22	Chrysene	448	1.422	BS

Notes:

a. Boiling points obtained from one or more of the following sources:
   - *CRC Handbook of Chemistry and Physics 57th Edition*
   - Merck Index 10th Edition 1983
   - Eastman Chemical Catalog 1988
   - Aldrich Chemical Catalog 1988-1989
   - EPA Method 1624/1625 Rev C
   - Chemical Hazardous Resource Information Service, DOT 1984
   - Int. Agency for Res. on Cancer, Monographs Vol. 1-42
   - Hazardous Substances Database, an online service of the National Library of Medicine

b. RRT values obtained from the following sources:
   - UP - Original Unidentified Peaks Study (Onstot 1987)
   - BS - FY82 Broad Scan Study (Stanley 1986a,b,c,d)



Note: Plot based on RRT data shown in Table 4.

Figure 2. Regression plot of semivolatiles with known boiling point vs. RRT.

Table 5

Semivolatile Compounds Which Were Manually Determined in the FY82 Data

No.	Compound Name	CAS No.
1	1-Amino-2-methylanthraquinone	82-28-0
2	2,4-D	94-75-7
3	2,4-Diaminoanisole	615-05-4
4	4,4'-Diaminodiphenyl ether	101-80-4
5	4,4'-Thiodianiline	139-65-1
6	4,6-Dinitro-o-cresol	534-52-1
7	4-Pentyl benzaldehyde	6853-57-2
8	Bis(2-ethylhexyl)adipate	103-23-1
9	Butyl glycol butyl phthalate	85-70-1
10	Chloramben	133-90-4
11	Chlorobenzilate	510-15-6
12	Decabromodiphenyl oxide	1163-19-5
13	Dicofol	115-32-2
14	Maneb	12427-38-2
15	Melamine	108-78-1
16	Michler's ketone	90-94-8
17	Picric acid	88-89-1
18	Propoxur	114-26-1
19	Tris(2,3-dibromopropyl) phosphate	126-72-7

Table 6

List of Volatile Target Analytes

No.	Compound Name	CAS No	Formula	Quan Ion (m/z)	B. Pt. (a)	RRT (b)
1	Acetone	67-64-1	C3.H6.O	58	57	0.315
2	Acetonitrile	75-05-8	C2.H3.N	41	82	0.552
3	Acrolein	107-02-8	C3.H4.O	55	53	0.293
4	Acrylic Acid	79-10-7	C3.H4.O2	72	141	1.730
5	Acrylonitrile	107-13-1	C3.H3.N	53	77	0.493
6	Allyl Chloride	107-05-1	C3.H5.Cl	76	45	0.259
7	2-Amyl furan	3777-69-3	C9.H14.O	138	na (c)	2.707
8	Bromoheptane (d)	629-04-9	C7.H15.Br	135	179	2.915
9	Bromopentane	110-53-2	C5.H11.Br	71	130	1.441
10	Butyl Acrylate	141-32-2	C7.H12.O2	73	145	1.841
11	tert-Butyl alcohol	75-65-0	C4.H10.O	59	82	0.552
12	n-Butyl Alcohol	71-36-3	C4.H10.O	56	117	1.144
13	sec-Butyl alcohol	78-92-2	C4.H10.O	59	100	0.819
14	1,2-Butylene oxide	106-88-7	C4.H8.O	42	63	0.359
15	Butyraldehyde	123-72-8	C4.H8.O	72	75	0.470
16	Carbon disulfide	75-15-0	C.S2	76	47	0.267
17	Carbon tetrachloride	56-23-5	C.CL4	117	77	0.493
18	Chloroprene	126-99-8	C4.H5.Cl	53	59	0.333
19	Cyclohexane	110-82-7	C6.H12	84	81	0.541
20	Diallate	2303-16-4	C10.H17.O.N.S.Cl2	234	150	1.985
21	1,2-Dibromoethane (Ethylene bromide)	106-93-4	C2.H4.Br2	107	131	1.470
22	1,2-Dichloroethane	107-06-2	C2.H4.Cl2	62	83	0.567
23	1,1-Dichloroethane	75-34-3	C2.H4.Cl2	63	57	0.319
24	1,2-Dichloroethylene	540-59-0	C2.H2.Cl2	96	48	0.274
25	1,2-Dichloropropane	78-87-5	C3.H6.Cl2	63	96	0.752
26	1,3-Dichloropropylene	542-75-6	C3.H4.CL2	75	104	0.889
27	1,4-Dioxane	123-91-1	C4.H8.O2	88	101	0.837
28	Epichlorohydrin	106-89-8	C3.H5.O.Cl	62	115	1.104
29	2-Ethoxyethanol	110-80-5	C4.H10.O2	72	135	1.570
30	Ethyl acrylate	140-88-5	C5.H8.O2	55	100	0.819
31	Ethyl chloroformate	541-41-3	C3.H5.O2.Cl	63	93	0.704
32	Ethyl isovalerate	108-64-5	C7.H14.O2	85	135	1.674
33	Ethyleneimine (Aziridine)	151-56-4	C2.H5.N	42	56	0.315
34	Freon 113	76-13-1	C2.Cl3.F3	151	na	0.223
35	1-Hexene	592-41-6	C6.H12	55	na	0.363
36	1-Iodopentane	628-17-1	C5.H11.I	198	na	2.150
37	Isobutyraldehyde	78-84-2	C4.H8.O	72	64	0.367
38	Isopropyl alcohol	67-63-0	C3.H8.O	59	83	0.553
39	Limonene (d)	138-86-3	C10.H16	136	178	2.89
40	2-Methoxyethanol	109-86-4	C3.H8.O2	45	124	1.30
41	Methyl acrylate	96-33-3	C4.H6.O2	85	81	0.54
42	Methyl ethyl ketone {2-Butanone}	78-93-3	C4.H8.O	72	80	0.53
43	Methyl iodide	74-88-4	C.H3.I	127	43	0.25
44	Methyl isobutyl ketone	108-10-1	C6.H12.O	100	118	1.16
45	Methyl methacrylate	80-62-6	C5.H8.O2	100	101	0.83
46	Methyl tert-butyl ether	1634-04-4	C5.H12.O	73	55	0.30
47	Methylene bromide	74-95-3	C.H2.Br2	172	97	0.76
48	N-Nitroso-N-ethylurea	759-73-9	C3.H7.O2.N3	74	103	0.87
49	2-Nitropropane	79-46-9	C3.H7.O2.N	43	120	1.21
50	p-Nitrosodiphenylamine	156-10-5	C12.H10.O.N2	198	145	1.81
51	Nonenes (1-Nonene)	124-11-8	C9.H18	56	148	1.93

Table 6

List of Volatile Target Analytes

No.	Compound Name	CAS No	Formula	Quan Ion (m/z)	B. Pt. (a)	RRT (b)
52	3-Octen-2-one	1669-44-9	C8.H14.O	126	na	2.959
53	Pentyl Alcohol (3-methyl-1-butanol)	123-51-3	C5.H12.O	70	137	1.622
54	Pentyl cyclohexane	4292-92-6	C11.H22	83	202	3.556
55	ß-Propiolactone	57-57-8	C3.H4.O2	42	162	2.363
56	Propionaldehyde	123-38-6	C3.H6.O	58	49	0.278
57	Propyleneimine	75-55-8	C3.H7.N	56	66	0.385
58	Pyridine	110-86-1	C5.H5.N	79	115	1.104
59	Quinone	106-51-4	C6.H4.O2	108	109	0.981
60	Trichloroethylene {Trichloroethene}	79-01-6	C2.H.Cl3	130	87	0.619
61	Vinyl acetate	108-05-4	C4.H6.O2	86	73	0.441

Notes:

a. Boiling points obtained from one or more of the following sources:
   CRC Handbook of Chemistry and Physics 57th Edition
   Merck Index 10th Edition 1983
   Eastman Chemical Catalog 1988
   Aldrich Chemical Catalog 1988-1989
   EPA Method 1624/1625 Rev C
   Chemical Hazardous Resource Information Service, DOT 1984
   Int. Agency for Res. on Cancer, Monographs Vol. 1-42
   Hazardous Substances Database, an online service of the
   National Library of Medicine

b. RRT used in target compound analysis of samples, based on 2-bromo-1-chloropropane internal standard.
   RRT was either predicted as described in the text or obtained from one of the following sources:
   "GC/MS Suitability Testing of RCRA Appendix VIII and Michigan List Analytes" (Lucas 1987)
   EPA Method 1624/25 (Rev. C, 1986)

c. Boiling point was unavailable.

d. Analyzed in both volatile and semivolatile fractions.

Table 7

List of Semivolatile Target Analytes

No.	Compound Name	CAS No	Formula	Quan Ion (m/z)	B. Pt. (a)	RRT (b)
1	2-Acetylaminofluorene	53-96-3	C15.H13.O.N	181	na (c)	1.328
2	1-Amino-2-methylanthraquinone	82-28-0	C15.H11.O2.N	237	na	na
3	2-Aminoanthraquinone	117-79-3	C14.H9.O2.N	223	na	1.699
4	4-Aminoazobenzene	60-09-3	C12.H11.N3	197	360	1.425
5	4-Aminobiphenyl	92-67-1	C12.H11.N	169	302	0.985
6	o-Anisidine	90-04-0	C7.H9.O.N	108	224	0.601
7	p-Anisidine	104-94-9	C7.H9.O.N	108	116	0.667
8	Anthracene	120-12-7	C14.H10	178	340	1.004
9	Benzal chloride	98-87-3	C7.H6.Cl2	125	205	0.530
10	Benzamide	55-21-0	C7.H7.O.N	105	228	0.613
11	Benzidine	92-87-5	C12.H12.N2	184	400	1.168
12	Benzo(a)anthracene	56-55-3	C18.H12	228	435	1.317
13	Benzo(b)fluoranthene	205-99-2	C20.H12	252	480	1.445
14	Benzo(a)pyrene	50-32-8	C20.H12	252	495	1.483
15	Benzoic acid	65-85-0	C7.H6.O2	105	249	0.647
16	Benzoic trichloride	98-07-7	C7.H5.Cl3	159	221	0.587
17	Benzoyl chloride	98-88-4	C7.H5.O.Cl	105	197	0.501
18	Benzyl chloride	100-44-7	C7.H7.Cl	126	179	0.438
19	Lindane (g-BHC)	58-89-9	C6.H6.Cl6	181	323	0.975
20	Biphenyl	92-52-4	C12.H10	154	256	0.668
21	Bis(2-chloro-1-methylethyl)ether	108-60-1	C6.H12.O.Cl2	121	187	0.466
22	Bis(2-chloroethyl)ether	111-44-4	C4.H8.O.Cl2	142	178	0.445
23	Bis(2-ethylhexyl)adipate	103-23-1	C22.H42.O4	129	na	na
24	Bromoheptane (d)	629-04-9	C7.H15.Br	135	179	0.438
25	Butyl glycol butyl phthalate	85-70-1	C18.H24.O6	149	na	1.275
26	Captan	133-06-2	C9.H8.O2.N.S.Cl3	264	na	1.165
27	Carbaryl	63-25-2	C12.H11.O2.N	144	na	1.076
28	Catechol	120-80-9	C6.H6.O2	110	246	0.678
29	Chloramben	133-90-4	C7.H5.O2.N.Cl2	205	na	na
30	p-Chloro-m-cresol	59-50-7	C7.H7.O.Cl	142	235	0.688
31	2-Chloroacetophenone (Tear gas)	532-27-4	C8.H7.O.Cl	105	244	0.669
32	Chlorobenzilate	510-15-6	C16.H14.O3.Cl2	251	na	na
33	Chlorothalonil	1897-45-6	C8.N2.Cl4	266	350	1.050
34	p-Cresidine	120-71-8	C8.H11.O.N	122	235	0.800
35	m-Cresol (m-methylphenol)	108-39-4	C7.H8.O	108	202	0.520
36	o-Cresol (o-methylphenol)	95-48-7	C7.H8.O	108	191	0.513
37	p-Cresol (p-methylphenol)	106-44-5	C7.H8.O	107	202	0.530
38	Cumene (isopropylbenzene)	98-82-8	C9.H12	105	152	0.292
39	Cumene hydroperoxide	80-15-9	C9.H12.O2	105	153	0.345
40	Cymene (isopropyltoluene)	99-87-6	C10.H14	119	175	0.348
41	2,4-D	94-75-7	C8.H6.O3.Cl2	162	na	na
42	Decabromodiphenyl oxide	1163-19-5	C12.O.Br10	800	na	na
43	Di-(2-ethylhexyl)phthalate (DEHP)	117-81-7	C24.H38.O4	149	386	1.405
44	2,4-Diaminoanisole	615-05-4	C7.H10.O.N2	123	na	na
45	4,4'-Diaminodiphenyl ether	101-80-4	C12.H12.O.N2	200	na	na
46	2,4-Diaminotoluene	95-80-7	C7.H10.N2	121	283	0.659
47	Dibenz(a,h)anthracene	53-70-3	C22.H14	278	525	1.677
48	Dibenzofuran	132-64-9	C12.H8.O	168	287	0.784
49	1,2-Dibromo-3-chloropropane	96-12-8	C3.H5.CL.Br2	157	196	0.526
50	3,3'-Dichlorobenzidine	91-94-1	C12.H10.N2.Cl2	252	na	1.310
51	Dichlorvos	62-73-7	C4.H7.O4.Cl2.P	109	140	0.653

Table 7

List of Semivolatile Target Analytes

No.	Compound Name	CAS No	Formula	Quan Ion (m/z)	B. Pt. (a)	RRT (b)
52	Dicofol	115-32-2	C14.H9.O.Cl5	139	na	1.448
53	Diethyl sulfate	64-67-5	C4.H10.O4.S	139	208	0.450
54	3,3'-Dimethoxybenzidine	119-90-4	C14.H16.O2.N2	244	na	1.364
55	2,4-Dimethyl phenol	105-67-9	C8.H10.O	122	212	0.582
56	Dimethyl sulfate	77-78-1	C2.H6.O4.S	125	189	0.473
57	4-Dimethylaminoazobenzene	60-11-7	C14.H15.N3	120	na	1.213
58	3,3'-Dimethylbenzidine (o-Tolidine)	119-93-7	C14.H16.N2	212	na	1.583
59	Dimethylcarbamyl chloride	79-44-7	C3.H6.O.N.Cl	107	168	0.398
60	4,6-Dinitro-o-cresol	534-52-1	C7.H6.O5.N2	121	na	0.852
61	2,4-Dinitrophenol	51-28-5	C6.H4.O5.N2	184	na	0.836
62	2,4-Dinitrotoluene	121-14-2	C7.H6.O4.N2	165	na	0.861
63	2,6-Dinitrotoluene	606-20-2	C7.H6.O4.N2	165	na	0.817
64	Diphenyl ether (1,1'-Oxybisbenzene)	101-84-8	C12.H10.O	170	259	na
65	2-Ethoxy benzaldehyde	613-69-4	C9.H10.O2	121	247	0.617
66	Fluometuron	2164-17-2	C10.H11.O.N2.F3	232	164	0.383
67	Hexachloro-1,3-butadiene	87-68-3	C4.Cl6	225	210	0.633
68	Hexachlorocyclopentadiene	77-47-4	C5.Cl6	237	239	0.720
69	Hexachloroethane	67-72-1	C2.Cl6	201	195	0.521
70	Hexamethylphosphoramide	680-31-9	C6.H18.O.N3.P	135	232	0.687
71	Hydroquinone	123-31-9	C6.H6.O2	110	286	0.669
72	Indeno(1,2,3-cd)pyrene	193-39-5	C22.H12	276	na	1.672
73	Isophorone	78-59-1	C9.H14.O	138	215	0.561
74	4,4'-Isopropylidenediphenol	80-05-7	C15.H16.O2	213	220	0.587
75	Limonene (d)	138-86-3	C10.H16	136	178	0.354
76	Maneb	12427-38-2	C4.H6.N2.S4.Mn	256	na	na
77	Melamine	108-78-1	C3.H6.N6	126	na	na
78	Methoxychlor	72-43-5	C16.H15.O2.Cl3	137	na	1.624
79	4,4'-Methylenebis(2-chloroaniline)	101-14-4	C13.H12.N2.Cl2	231	na	1.337
80	4,4'-Methylenebis(N,N-dimethyl)benzen	101-61-1	C17.H22.N2	192	390	1.193
81	4,4'-Methylenedianiline	101-77-9	C13.H14.N2	198	398	2.025
82	Michler's ketone	90-94-8	C17.H20.O.N2	148	na	na
83	N,N-Dimethylaniline	121-69-7	C8.H11.N	120	193	0.488
84	N-Nitrosodi-n-butylamine	924-16-3	C8.H18.O.N2	116	243	0.667
85	N-Nitrosodi-n-propylamine	621-64-7	C6.H14.O.N2	130	206	0.524
86	N-Nitrosodiphenylamine	86-30-6	C12.H10.O.N2	168	na	0.923
87	N-Nitrosomorpholine	59-89-2	C4.H8.O2.N2	116	224	0.526
88	N-Nitrosopiperidine	100-75-4	C5.H10.O.N2	114	215	0.565
89	a-Naphthylamine	134-32-7	C10.H9.N	143	301	0.797
90	ß-Naphthylamine	91-59-8	C10.H9.N	143	306	0.863
91	5-Nitro-o-anisidine	99-59-2	C7.H8.O3.N2	168	na	1.192
92	Nitrobenzene	98-95-3	C6.H5.O2.N	123	211	0.536
93	4-Nitrobiphenyl	92-93-3	C12.H9.O2.N	152	325	1.041
94	Nitrofen	1836-75-5	C12.H7.O3.N.Cl2	283	na	1.240
95	2-Nitrophenol	88-75-5	C6.H5.O3.N	139	215	0.567
96	4-Nitrophenol	100-02-7	C6.H5.O3.N	139	279	0.852
97	Octachloronaphthalene	2234-13-1	C10.Cl8	404	440	1.372
98	Parathion	56-38-2	C10.H14.O5.N.S.P	109	375	1.123
99	4-Pentyl benzaldehyde	6853-57-2	C12.H16.O	120	na	n
100	2-Phenyl phenol (o-Phenol phenol)	90-43-7	C12.H10.O	170	286	0.77
101	p-Phenylenediamine	106-50-3	C6.H8.N2	108	267	0.75
102	Phthalic anhydride	85-44-9	C8.H4.O3	104	285	0.81

Table 7

List of Semivolatile Target Analytes

No.	Compound Name	CAS No	Formula	Quan Ion (m/z)	B. Pt. (a)	RRT (b)
103	Picric acid	88-89-1	C6.H3.O7.N3	229	na	n
104	Propane sulfone	1120-71-4	C3.H6.O3.S	122	180	0.44
105	Propoxur	114-26-1	C11.H15.O3.N	110	na	0.88
106	Quinoline	91-22-5	C9.H7.N	129	238	0.64
107	Quintozene (Pentachloronitrobenzene)	82-68-8	C6.O2.N.CL5	295	328	1.20
108	Safrole	94-59-7	C10.H10.O2	162	233	0.59
109	Styrene oxide	96-09-3	C8.H8.O	120	194	0.49
110	Terephthalic acid	100-21-0	C8.H6.O4	149	288	0.82
111	Tetrachlorvinphos	961-11-5	C10.H9.O4.Cl4.P	329	na	1.19
112	4,4'-Thiodianiline	139-65-1	C12.H12.N2.S	216	na	n
113	Toluene-2,4-diisocyanate	584-84-9	C9.H6.O2.N2	174	251	0.72
114	o-Toluidine	95-53-4	C7.H9.N	106	201	0.51
115	o-Toluidine hydrochloride	636-21-5	C7.H10.N.Cl	106	242	0.66
116	Trifluralin	1582-09-8	C13.H16.O4.N3.F3	306	na	0.94
117	1,2,4-Trimethylbenzene	95-63-6	C9.H12	105	170	0.32
118	Tris(2,3-dibromopropyl) phosphate	126-72-7	C9.H15.O4.Br6.P	201	na	n
119	2,6-Xylidine	87-62-7	C8.H11.N	106	213	0.47
120	Zineb	12122-67-7	C4.H6.N2.S4.ZN	144	na	1.98

Notes:

a. Boiling points obtained from one or more of the following sources:
   CRC Handbook of Chemistry and Physics 57th Edition
   Merck Index 10th Edition 1983
   Eastman Chemical Catalog 1988
   Aldrich Chemical Catalog 1988-1989
   EPA Method 1624/1625 Rev C
   Chemical Hazardous Resource Information Service, DOT 1984
   Int. Agency for Res. on Cancer, Monographs Vol. 1-42
   Hazardous Substances Database, an online service of the
   National Library of Medicine

b. RRT used in target compound analysis of samples, based on d10-anthracene internal standard.
   RRT was either predicted as described in the text or obtained from one of the following sources:
   "GC/MS Suitability Testing of RCRA Appendix VIII and Michigan List Analytes" (Lucas 1987)
   EPA Method 1624/25 (Rev. C, 1986)

c. Boiling point was unavailable.

d. Analyzed in both volatile and semivolatile fractions.

e. RRT was unavailable. Determination for this compound was performed via manual examination of characteristic ion plots.

Table 8

SARA Compounds Eliminated from Consideration as Target Analytes

No.	Compound Name	CAS No.	Comments
1	Acetaldehyde	75-07-0	Boiling pt too low for VOA detn. (a)
2	Acetamide	60-35-5	Mol. wt. too low for SMV detn. (b)
3	Acrylamide	79-06-1	Polar (c)
4	Aldrin	309-00-2	Broad scan target analyte (d)
5	Aluminum (fume or dust)	7429-90-5	Inorganic
6	Aluminum Oxide	1344-28-1	Inorganic
7	Ammonia	7664-41-7	Inorganic
8	Ammonium nitrate (solution)	6484-52-2	Inorganic
9	Ammonium sulfate (solution)	7783-20-2	Inorganic
10	Aniline	62-53-3	Mol. wt. too low for SMV detn.
11	o-Anisidine hydrochloride	134-29-2	Redundant (see Anisidine)
12	Antimony	7440-36-0	Inorganic
13	Arsenic	7440-38-2	Inorganic
14	Asbestos (friable)	1332-21-4	Inorganic
15	Barium	7440-39-3	Inorganic
16	Benzene	71-43-2	Broad Scan target analyte
17	Benzoyl peroxide	94-36-0	Unstable
18	Beryllium	7440-41-7	Inorganic
19	∂-BHC	319-86-8	Broad Scan Target Analyte
20	a-BHC	319-84-6	Broad Scan Target Analyte
21	ß-BHC	319-85-7	Broad Scan Target Analyte
22	Bis(chloromethyl)ether	542-88-1	Unstable (c)
23	Bromoform	75-25-2	Broad scan target analyte
24	Bromomethane	74-83-9	Boiling pt too low for VOA detn.
25	1,3-Butadiene	106-99-0	Boiling pt too low for VOA detn.
26	Butyl benzyl phthalate	85-68-7	Broad Scan Target Analyte
27	C.I. Acid Blue 9, diammonium salt	2650-18-2	Nonvolatile, dye
28	C.I. Acid Blue 9, disodium salt	3844-45-9	Nonvolatile, dye
29	C.I. Acid Green 3	4680-78-8	Nonvolatile, dye
30	C.I. Basic Green 4	569-64-2	Nonvolatile, dye
31	C.I. Basic Red 1	989-38-8	Nonvolatile, dye
32	C.I. Direct Black 38	1937-37-7	Nonvolatile, dye
33	C.I. Direct Blue 6	2602-46-2	Nonvolatile, dye
34	C.I. Direct Brown 95	16071-86-6	Nonvolatile, dye
35	C.I. Disperse Yellow 3	2832-40-8	Nonvolatile, dye
36	C.I. Food Red 15	81-88-9	Nonvolatile, dye
37	C.I. Food Red 5	3761-53-3	Nonvolatile, dye
38	C.I. Solvent Orange 7	3118-97-6	Nonvolatile, dye
39	C.I. Solvent Yellow 14	842-07-9	Nonvolatile, dye
40	C.I. Solvent Yellow 3	97-56-3	Nonvolatile, dye
41	C.I. Solvent Yellow 34	492-80-8	Nonvolatile, dye
42	C.I. Vat Yellow 4	128-66-5	Nonvolatile, dye
43	Cadmium	7440-43-9	Inorganic
44	Calcium cyanamide	156-62-7	Inorganic
45	Carbonyl sulfide	463-58-1	BP too low for detn. (a)
46	Chlordane	57-74-9	Broad scan target analyte
47	Chlorine	7782-50-2	Inorganic

Table 8

SARA Compounds Eliminated from Consideration as Target Analytes

No.	Compound Name	CAS No.	Comments
48	Chlorine dioxide	10049-04-4	Inorganic
49	Chloroacetic acid	79-11-8	Mol. wt. too low for SMV detn.
50	Chlorobenzene	108-90-7	Broad scan target analyte
51	Chlorodibromomethane	124-48-1	Broad scan target analyte
52	Chloroethane	75-00-3	Boiling pt too low for VOA detn.
53	Chloroform	67-66-3	Broad scan target analyte
54	Chloromethane	74-87-3	Boiling pt too low for VOA detn.
55	Chloromethyl methyl ether	107-30-2	Unstable (c)
56	Chromium	7440-47-3	Inorganic
57	Chrysene	218-01-9	Broad scan target analyte
58	Cobalt	7440-48-4	Inorganic
59	Copper	7440-50-8	Inorganic
60	Cresols, Mixed	1319-77-3	Isomers analyzed individually
61	Cupferron	135-20-6	Thermolabile (c)
62	Cyanide	57-12-5	Inorganic
63	4,4'-DDD	72-54-8	Broad Scan Target Analyte
64	4,4'-DDE	72-55-9	Broad Scan Target Analyte
65	4,4'-DDT	50-29-3	Broad Scan Target Analyte
66	Di-n-octyl phthalate	117-84-0	Broad scan target analyte
67	2,4-Diaminoanisole sulfate	39156-41-7	Redundant (see Diaminoanisole)
68	Diaminotoluene (mixed isomers)	25376-45-8	Isomers analyzed individually
69	Diazomethane	334-88-3	Unstable
70	Dibutyl phthalate {Di-n-butyl phthalate}	84-74-2	Broad scan target analyte
71	1,2-Dichlorobenzene	95-50-1	Broad scan target analyte
72	1,4-Dichlorobenzene	106-46-7	Broad scan target analyte
73	1,3-Dichlorobenzene	541-73-1	Broad scan target analyte
74	Dichlorobenzenes (mixed isomers)	25321-22-6	Broad scan target analyte
75	Dichlorobromomethane	75-27-4	Broad scan target analyte
76	Dichlorodifluoromethane (Freon 12)	75-71-8	Boiling pt too low for VOA detn.
77	Dichloromethane {Methylene Chloride}	75-09-2	Broad scan target analyte
78	2,4-Dichlorophenol	120-83-2	Broad Scan Target Analyte
79	Dieldrin	60-57-1	Broad Scan Target Analyte
80	Diepoxybutane	1464-53-5	Mol. wt. too low for SMV detn.
81	Diethanolamine	111-42-2	Mol. wt. too low for SMV detn.
82	Diethyl phthalate	84-66-2	Broad scan target analyte
83	1,1-Dimethyl hydrazine	57-14-7	Basic, polar (c)
84	Dimethyl phthalate	131-11-3	Broad Scan target analyte
85	p-Dioxin	1745-01-6	No available reference mass spectrum
86	1,2-Diphenyl hydrazine	122-66-7	Thermolabile (c)
87	Endrin	72-20-8	Readily converted in endrin aldehyde
88	Endrin Aldehyde	7421-93-4	Broad Scan target analyte
89	Ethylbenzene	100-41-4	Broad scan target analyte
90	Ethylene	74-85-1	Boiling pt too low for VOA detn.
91	Ethylene glycol	107-21-1	Mol. wt. too low for SMV detn.
92	Ethylene oxide {Oxirane}	75-21-8	Boiling pt too low for VOA detn.
93	Ethylene thiurea	96-45-7	Mol. wt. too low for SMV detn.
94	Fluoranthene	206-44-0	Broad Scan Target Analyte

Table 8

SARA Compounds Eliminated from Consideration as Target Analytes

No.	Compound Name	CAS No.	Comments
95	Fluorotrichloromethane (Freon 11)	75-69-4	Boiling pt too low for VOA detn.
96	Formaldehyde	50-00-0	Polymerizes (c)
97	Heptachlor	76-44-8	Broad scan target analyte
98	Heptachlor Epoxide	1024-57-3	Broad Scan Target Analyte
99	Hexachlorobenzene	118-74-1	Broad scan target analyte
100	Hexachloronaphthalene	1335-87-1	No available reference mass spectrum
101	Hydrazine	302-01-2	Unsuitable to method (c)
102	Hydrazine sulfate	10034-93-2	Inorganic
103	Hydrochloric acid	7647-01-0	Inorganic
104	Hydrogen cyanide	74-90-8	Inorganic
105	Hydrogen fluoride	7664-39-3	Inorganic
106	Lead	7439-92-1	Inorganic
107	Maleic anhydride	108-31-6	Mol. wt. too low for SMV detn.
108	Manganese	7439-96-5	Inorganic
109	Mercury	7439-97-6	Inorganic
110	Methanol	67-56-1	Mol. wt. too low for VOA detn.
111	Methyl hydrazine	60-34-4	Basic, polar (c)
112	Methyl isocyanate	624-83-9	Boiling pt too low for VOA detn.
113	Methylenebis(phenylisocyanate) (MBI)	101-68-8	No available reference mass spectrum
114	Molybdenum trioxide	1313-27-5	Inorganic
115	Mustard gas	505-60-2	No available reference mass spectrum
116	N-Nitroso-N-methylurea	684-93-5	Mol. wt. too low for SMV detn.
117	N-Nitrosodiethylamine	55-18-5	Mol. wt. too low for SMV detn.
118	N-Nitrosodimethylamine	62-75-9	Mol. wt. too low for SMV detn.
119	N-Nitrosomethylvinylamine	4549-40-0	Mol. wt. too low for SMV detn.
120	N-Nitrosonornicotine	16543-55-8	No available reference mass spectrum
121	Naphthalene	91-20-3	Broad scan target analyte
122	Nickel	7440-02-0	Inorganic
123	Nitric acid	7697-37-2	Inorganic
124	Nitrilotriacetic acid	139-13-9	Acid
125	Nitrogen mustard	51-75-2	Unsuitable to method
126	Nitroglycerin	55-63-0	Inorganic
127	Osmium tetroxide	20816-12-0	Inorganic
128	Pentachlorophenol (PCP)	87-86-5	Broad Scan target analyte
129	Peracetic acid	79-21-0	Inorganic
130	Phenanthrene	85-01-8	Broad Scan Target Analyte
131	Phenol	108-95-2	Mol. wt. too low for SMV detn.
132	Phosgene	75-44-5	Inorganic
133	Phosphoric acid	7664-38-2	Inorganic
134	Phosphorus (yellow or white)	7723-14-0	Inorganic
135	Polychlorinated biphenyls (PCB'S)	1336-36-3	Broad scan target analyte
136	Propylene	115-07-1	Boiling pt too low for VOA detn.
137	Propylene oxide	75-56-9	Boiling pt too low for VOA detn.
138	Saccharin	81-07-2	Non-volatile, polar (c)
139	Selenium	7782-49-2	Inorganic
140	Silver	7440-22-4	Inorganic
141	Sodium hydroxide (solution)	1310-73-2	Inorganic

Table 8

SARA Compounds Eliminated from Consideration as Target Analytes

No.	Compound Name	CAS No.	Comments
142	Sodium sulfate (solution)	7757-82-6	Inorganic
143	Styrene	100-42-5	Broad scan target analyte
144	Sulfuric acid	7664-93-9	Inorganic
145	1,1,2,2-Tetrachloroethane	79-34-5	Broad scan target analyte
146	Tetrachloroethylene {Tetrachloroethene}	127-18-4	Broad scan target analyte
147	Thallium	7440-28-0	Inorganic
148	Thioacetamide	62-55-5	Mol. wt. too low for SMV detn.
149	Thiourea	62-56-6	Thermolabile, polar
150	Thorium dioxide	1314-20-1	Inorganic
151	Titanium dioxide	13463-67-7	Inorganic
152	Titanium tetrachloride	7550-45-0	Inorganic
153	Toluene	108-88-3	Broad scan target analyte
154	Toluene-2,6-diisocyanate	91-08-7	No available reference mass spectrum
155	Toxaphene	8001-35-2	Broad scan target analyte
156	Triaziquinone	68-76-8	No available reference mass spectrum
157	Trichlorfon	52-68-6	Thermolabile (c)
158	1,2,4-Trichlorobenzene	120-82-1	Broad scan target analyte
159	1,1,1-Trichloroethane	71-55-6	Broad scan target analyte (c)
160	1,1,2-Trichloroethane	79-00-5	Broad scan target analyte
161	2,4,6-Trichlorophenol	88-06-2	Broad Scan target analyte
162	2,4,5-Trichlorophenol	95-95-4	Broad Scan target analyte
163	Urethane (Ethyl carbamate)	51-79-6	Mol. wt. too low for SMV detn.
164	Vanadium (fume or dust)	7440-62-2	Inorganic
165	Vinyl bromide	593-60-2	Boiling pt too low for VOA detn.
166	Vinyl chloride	75-01-4	Boiling pt too low for VOA detn.
167	Vinylidene chloride {1,1-Dichloroethene}	75-35-4	Boiling pt too low for VOA detn.
168	o-Xylene	95-47-6	Broad scan target analyte
169	p-Xylene	106-42-3	Broad scan target analyte
170	m-Xylene	108-38-3	Broad scan target analyte
171	Xylene (mixed isomers)	1330-20-7	Broad scan target analyte
172	Zinc	7440-66-6	Inorganic

Notes:

a. Compounds with boiling points lower than ca. 40° C were not detectable in VOA composites.

b. Compounds with molecular weight less than 110 amu were not detectable in SMV composites.

c. "GC/MS Suitability Testing of RCRA Appendix VIII and Michigan List Analytes", EPA/600/4-87/024 Aug. 1987

d. Previously quantitated as part of the Broad Scan Study (Stanley 1986a, b, c, d).

E. Target Compound Analysis

Execution of the target compound analysis proceeded in four steps:

1. Creation of TCA quantitation libraries.

2. Application of TCA procedure to FY82 data.

3. Manual review of TCA output.

4. Transfer of TCA results to a database.

As previously stated, the TCA procedure required that the RRT and reference mass spectrum be placed in a special quantitation library which the TCA procedure uses in the search routine. For this study, two separate libraries were constructed; one each for the volatile and semivolatile TCA analytes, respectively. In addition to the information above, other parameters used to control the searching routine were entered into the quantitation libraries at this time, including search window half-widths and minimum FIT thresholds. Based on the standard deviation of error calculated for the RRT vs. boiling point regression plots, a search window half-width of 45 s and 60 s was initially used for the volatiles and semivolatiles, respectively. This provided sufficiently broad windows such that any errors in RRT prediction would not result in a compound being missed by the searching procedure. If a compound was identified in a sample during the course of analysis, the search window half-width was reduced to 20 s around the retention time from the predicted observed RRT for all subsequent analyses to reduce the search time of the TCA program. A minimum FIT of 750 and 900 (based on a weighted comparison to the reference mass spectrum and ranging from 0 for no similarity between spectra to 1000 for a perfect match between spectra) was used for the VOA and SMV analytes, respectively.

The data set used in this study consisted of composited human adipose tissue specimens prepared from the NHATS repository and were originally analyzed as part of a broad scan study. The composite samples were originally analyzed by HRGC/MS for volatiles and semivolatiles during the period from April 1984 to July 1984 (Stanley 1986a, Stanley 1986b). The resulting HRGC/MS datafiles were generated from the analysis of 46 volatiles, 44 semivolatiles from the 6% Florisil cleanup fraction, and 46 semivolatiles from the 15/50% cleanup fraction. Within each of these categories, there were 12, 15, and 17 samples in the 0-14, 15-44, and 45+ age groups for the 6% semivolatiles, and 12, 17, and 17 samples in the 0-14, 15-44 and 45+ age groups for the volatiles and 15/50% semivolatiles, respectively.

In addition to the samples above, six semivolatile method blanks, six Florisil blanks (corresponding to three of each type for the 6% and 15/50% Florisil fractions, respectively), and 11 volatile purge vessel blanks were also analyzed using the same procedure.

Application of the TCA procedure to the FY82 data was performed on a Finnigan/MAT Incos data system using the AutoQuan TCA software provided. At the end of each TCA analysis, two documents were generated by the TCA program:

a search summary report containing information about the success of the search procedure, and a quantitation report containing the semiquantitative results of the search. Results of each TCA analysis were manually reviewed to verify the accuracy of the data. The manual review consisted of verifying each compound identification via manual comparison of the unknown mass spectrum to the reference spectrum. The TCA search summary provided the FIT values associated with each positive identification. However, the use of FIT as the primary criterion for identification often did not provide sufficient selectivity when the target compound was searched within a retention window containing large nontarget peaks. As a result, many false positive identifications were made by TCA. This was especially true for targets which did not have distinctive mass spectra. The difficulty of identifying target compounds with non-distinctive mass spectra is discussed in Section V.

Compound identifications were also checked against the summary reports generated in the original unidentified peaks study. This check proved useful in identifying persistent misidentifications by TCA due to interference by nontarget peaks as described above. For example, the TCA procedure consistently identified the compound acetonitrile in most of the volatile composites, but a check of the associated unidentified peaks summary report indicated that the same peak was consistently identified as pentanal in the original study. Comparison of the two reference mass spectra revealed that these compounds exhibit many of the same ion masses, which resulted in the false positive identification of acetonitrile whenever pentanal was present. A TCA target identification was not rejected solely on the basis of a peak's previous identification in the unidentified peaks study. However, prior identification of a peak was seen as an indicator for the need for additional checking in the form of more extensive mass spectral enhancement and background subtraction techniques.

As indicated previously, a few compounds could not be analyzed using the automated TCA procedure because no retention information could be found. These compounds were analyzed by examining the mass chromatograms of the three major ions for each compound for possible occurrences based on relative abundance measurements of observed peaks. Only one compound, bis(ethylhexyl)-adipate, was found using this method.

The results of all TCA analyses were transferred to an Apple Macintosh and were imported into a database (Fourth Dimension, Acius, Inc.) for final processing and report generation.

F. GC/MS Analysis of Authentic Standards

After compiling the target compound analysis results into lists of tentatively identified compounds, authentic compound material was procured and composite standard solutions were prepared. All of the tentatively identified compounds were obtained from commercial sources, with the exception of pentyl benzaldehyde, which was not delivered in time to be included in this portion of the study. A set of authentic compound solutions ranging from 10 to 400 ppm was prepared for each of the three fraction types: volatiles, 6% semivolatiles, and 15/50% semivolatiles. Gas chromatograph and mass

spectrometer parameters were adjusted to match those used in the original analysis as closely as possible, with the following exceptions:

- A mass scanning range of 45 to 400 amu was used for the semivolatile analysis;
- A 15-m DB5 megabore FSCC column was used in place of the 30-m DB5 narrow bore for the volatile analysis;
- A Finnigan/MAT 312 magnetic sector mass spectrometer was used instead of the Finnigan 4500 mass spectrometer for the volatile analysis; and
- No heated vessel was used in the sample introduction setup for the volatile analysis. This portion of the setup was only used to purge the adipose of the volatiles, which then passed through an unheated purge tower filled with 1 to 5 mL of water. In the analysis of the volatile authentic standards, the appropriate amount of volatile standard solution was injected into a 5-mL syringe of volatile-free water, which was immediately transferred directly into the unheated purge tower.

GC program parameters were adjusted so that the retention times of the authentic standards would match the retention times of the original analysis as closely as possible. In order to accomplish this, composite solutions containing some of the original broad scan target analytes were run and compared with their original retention times. Table 9 shows the comparison between the RRTs of selected broad scan target analytes as seen in both the original 1984 analysis and this analysis (1989). Fairly close agreement was achieved for the volatile compounds, with a percent relative difference ranging from -1% to 4%. Agreement was not as good as for the semivolatiles, although there did appear to be a trend in the percent relative RRT differences, with 1989 RRTs being higher than 1984 RRTs at the low end of the retention range and lower than the 1984 RRTs at the high end of the retention range. A linear regression of the 1984 vs. 1989 semivolatile data was then plotted and later used to adjust the RRT values of the authentic standards of tentatively identified compounds so that they would more closely approximate the RRTs that they would have had under 1984 conditions.

When GC parameters had been optimized to match the original analysis RRTs, the authentic standard solutions were analyzed. Two standards corresponding to 100 and 400 ng of each authentic compound were analyzed for each of the three standard sets. Average relative response factor (RRf) and RRT values were determined from these authentic standards analyses. The semivolatile RRT values were then adjusted to match 1984 conditions using the 1984 vs. 1989 broad scan RRT regression analysis, as previously described. The volatile RRT values were not adjusted since there was already good agreement between the 1989 RRTs and the 1984 RRTs.

Table 9

RRT Comparison of Selected Broad Scan Target Analytes
1984 Analysis vs 1989 Analysis

Volatiles

Compound Name	RRT[a] .(1984)	RRT[a] .(1989)	Δ RRT (%)	RRf[b] .(1989)
Bromochloromethane	.408	.404	-1	.423
1,1,1-Trichloroethane	.462	.481	4	.368
Benzene	.498	.512	3	1.148
Tetrachloroethene	1.256	1.232	-2	.379
Dibromochloromethane	1.162	1.126	-3	.361
1,1,2-Trichloroethane	.996	.986	-1	.275
Toluene	.949	.961	1	1.045
Chlorobenzene	1.531	1.509	-1	.821
Ethylbenzene	1.653	1.649	0	.410
Bromoform	1.823	1.814	0	.272
1,1,2,2-Tetrachloroethane	2.061	2.081	1	.473

Semivolatiles

Compound Name	RRT[a] .(1984)	RRT[a] .(1989)	Δ RRT (%)	RRf[b] .(1989)
1,4-Dichlorobenzene	0.35	0.4	14	1.184
Naphthalene	0.49	0.54	11	1.731
Fluorene	0.84	0.87	3	.938
Hexachlorobenzene	0.94	0.96	2	.264
Fluoranthene	1.19	1.18	-1	1.200
Butyl benzyl phthalate	1.36	1.32	-3	.513
Chrysene	1.43	1.39	-3	.905
Bis(2-ethylhexyl) phthalate	1.46	1.41	-4	.782
Dibenz(a,h)anthracene	1.84	1.8	-2	.568

Notes:

a. RRT values calculated vs 2-Bromo-1-chloropropane for volatile compounds and d10-Anthracene for semivolatile compounds.

b. RRf values calculated vs 2-Bromo-1-chloropropane for volatile compounds and d10-Anthracene for semivolatile compounds.

The authentic compound RRT values were compared to the respective tentatively identified peak RRTs. If the RRT of the authentic standard compound fell within the range of the RRTs observed in the composites, and if the mass spectra of the authentic and tentatively identified peaks were identical, the compound was considered positively identified. Some exceptions were made if a compound fell slightly outside the RRT range of observed hits if there was a compelling reason to do so, such as a very high mass spectral similarity between the authentic and observed spectra, or if the authentic RRT was only slightly outside the range of RRTs observed in the adipose composites. This was done to compensate for both the rather broad variation of RRTs which were actually observed in the original analysis and for the unavoidable minor differences in GC conditions between the original analysis and the authentic standards analysis.

IV. RESULTS

Application of the target compound analysis procedure to the FY82 composites as described above resulted in the following tables of results. Tables 10 through 12 present the target compounds identified in the volatile, 6% semivolatile Florisil, and 15/50% semivolatile Florisil 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 name and CAS Registry No. columns are derived from the compound's respective source listing. In cases where a compound name was reported differently in the source listings, the naming precedence is Title III > Title 110 > ECAD. The remaining columns show the frequency of occurrence of the listed compounds within the three tested age groups.

Tables 13 and 14 show the lists of compounds which were searched in the FY82 composites but which were not observed in the volatile and semivolatile sample fractions, respectively.

Additional tables detailing the the occurrences of compounds identified in the FY82 data and their relative responses are presented in Appendices A through G. Appendices A through C show the quantitative results for each identified compound in the volatile, 6% and 15/50% semivolatile fractions, respectively. Appendices D through F show occurrences of target compounds as a function of census region and census division for the volatile, 6% and 15/50% semivolatile fractions, respectively. Appendix G presents representative hardcopies of library mass spectral comparisons for each target compound identified in the FY82 data.

Table 10

SARA/ECAD Compounds Identified in FY82 Adipose Composites

VOA Fraction

No.	Name	CAS No.	Frequency of Occurrence				
			Total [a]	0-14 [b]	15-44	45+	Blanks [c]
1	2-Amyl furan	3777-69-3	46	12	18	16	1
2	Bromoheptane	629-04-9	4	2	1	1	0
3	Bromopentane	110-53-2	3	2	1	0	0
4	Butyraldehyde	123-72-8	45	11	17	17	0
5	Ethyl isovalerate	108-64-5	44	11	17	16	0
6	1-Iodopentane	628-17-1	35	9	14	12	0
7	Isobutyraldehyde	78-84-2	43	11	16	16	0
8	Limonene	138-86-3	46	12	18	16	0
9	Nonenes (1-Nonene)	124-11-8	46	12	17	17	6
10	3-Octen-2-one	1669-44-9	45	12	18	15	0
11	Pentyl Alcohol	123-51-3	38	7	15	16	0
12	Pentyl cyclohexane	4292-92-6	10	1	5	4	0
13	Trichloroethylene	79-01-6	20	3	8	9	0

Notes:

a. Frequency determined from a total of 46 composite samples.

b. 0-14 = Samples collected from persons between the ages of 0-14 years.
15-44 = Samples collected from persons between the ages of 15-44 years.
45+ = Samples collected from persons above 45 years of age.

c. A total of 11 vessel blanks were analyzed for volatile compounds.

Table 11

SARA/ECAD Compounds Identified in FY82 Adipose Composites

6% SMV Fraction

No.	Name	CAS No.	Frequency of Occurrence				
			Total [a]	0-14 [b]	15-44	45+	Blanks [c]
1	Anthracene	120-12-7	1	0	1	0	0
2	Biphenyl	92-52-4	9	2	2	5	0
3	Cymene (isopropyltoluene)	99-87-6	41	11	15	15	0
4	Dibenzofuran	132-64-9	3	1	2	0	0
5	Diphenyl ether (1,1'-Oxybisbenzene)	101-84-8	40	11	14	15	0
6	Limonene	138-86-3	41	11	15	15	0
7	Safrole	94-59-7	4	0	1	3	0
8	1,2,4-Trimethylbenzene	95-63-6	42	11	15	16	4
9	2,6-Xylidine	87-62-7	11	0	1	10	0

[a] Frequency determined from a total of 44 composite samples.
[b] 0-14 = Samples collected from persons between the ages of 0-14 years.
15-44 = Samples collected from persons between the ages of 15-44 years.
45+ = Samples collected from persons above 45 years of age.
[c] A total of six blanks were analyzed for 6% semivolatile compounds.

Table 12

SARA/ECAD Compounds Identified in FY82 Adipose Composites

15/50% SMV Fraction

No.	Name	CAS No.	Frequency of Occurrence				
			Total [a]	0-14 [b]	15-44	45+	Blanks [c]
1	Bis(2-ethylhexyl)adipate	103-23-1	8	1	4	3	0
2	Butyl glycol butyl phthalate	85-70-1	8	0	4	4	0
3	Carbaryl	63-25-2	1	0	0	1	0
4	o-Cresol (o-methylphenol)	95-48-7	38	10	14	14	0
5	m,p-Cresol (m,p-methylphenol)	106-44-5	43	11	16	16	0
6	Di-(2-ethylhexyl)phthalate (DEHP)	117-81-7	42	10	15	17	4
7	2,4-Diaminotoluene	95-80-7	20	1	9	10	0
8	2-Ethoxy benzaldehyde	613-69-4	6	4	1	1	0
9	4-Pentyl benzaldehyde [d]	6853-57-2	9	5	1	3	0
10	2-Phenyl phenol (o-Phenol phenol)	90-43-7	22	5	6	11	0

[a] Frequency determined from a total of 46 composite samples.
[b] 0-14 = Samples collected from persons between the ages of 0-14 years.
15-44 = Samples collected from persons between the ages of 15-44 years.
45+ = Samples collected from persons above 45 years of age.
[c] A total of six blanks were analyzed for 15/50% semivolatile compounds.
[d] Identification of this compound was not confirmed by GC/MS analysis of authentic standard material.

Table 13

Volatile Compounds Not Detected in FY82 Adipose Composites

No.	Compound Name	CAS No.	No.	Compound Name	CAS No.
1	Acetone	67-64-1	25	2-Ethoxyethanol	110-80-5
2	Acetonitrile	75-05-8	26	Ethyl acrylate	140-88-5
3	Acrolein	107-02-8	27	Ethyl chloroformate	541-41-3
4	Acrylic Acid	79-10-7	28	Ethyleneimine (Aziridine)	151-56-4
5	Acrylonitrile	107-13-1	29	Freon 113	76-13-1
6	Allyl Chloride	107-05-1	30	1-Hexene	592-41-6
7	Butyl Acrylate	141-32-2	31	Isopropyl alcohol	67-63-0
8	n-Butyl alcohol	71-36-3	32	2-Methoxyethanol	109-86-4
9	tert-Butyl alcohol	75-65-0	33	Methyl acrylate	96-33-3
10	sec-Butyl alcohol	78-92-2	34	Methyl ethyl ketone	78-93-3
11	1,2-Butylene oxide	106-88-7	35	Methyl iodide	74-88-4
12	Carbon disulfide	75-15-0	36	Methyl isobutyl ketone	108-10-1
13	Carbon tetrachloride	56-23-5	37	Methyl methacrylate	80-62-6
14	Chloroprene	126-99-8	38	Methyl tert-butyl ether	1634-04-4
15	Cyclohexane	110-82-7	39	Methylene bromide	74-95-3
16	Diallate	2303-16-4	40	N-Nitroso-N-ethylurea	759-73-9
17	1,2-Dibromoethane (Ethylene bromide)	106-93-4	41	2-Nitropropane	79-46-9
18	1,2-Dichloroethane	107-06-2	42	p-Nitrosodiphenylamine	156-10-5
19	1,1-Dichloroethane	75-34-3	43	Propionaldehyde	123-38-6
20	1,2-Dichloroethylene	540-59-0	44	ß-Propiolactone	57-57-8
21	1,2-Dichloropropane	78-87-5	45	Propyleneimine	75-55-8
22	1,3-Dichloropropylene	542-75-6	46	Pyridine	110-86-1
23	1,4-Dioxane	123-91-1	47	Quinone	106-51-4
24	Epichlorohydrin	106-89-8	48	Vinyl acetate	108-05-4

Table 14

Semivolatile Compounds Not Detected in FY82 Adipose Composites

No.	Compound Name	CAS No.	No.	Compound Name	CAS No.
1	2-Acetylaminofluorene	53-96-3	52	Fluometuron	2164-17-2
2	1-Amino-2-methylanthraquinone	82-28-0	53	Hexachloro-1,3-butadiene	87-68-3
3	2-Aminoanthraquinone	117-79-3	54	Hexachlorocyclopentadiene	77-47-4
4	4-Aminoazobenzene	60-09-3	55	Hexachloroethane	67-72-1
5	4-Aminobiphenyl	92-67-1	56	Hexamethylphosphoramide	680-31-9
6	o-Anisidine	90-04-0	57	Hydroquinone	123-31-9
7	p-Anisidine	104-94-9	58	Indeno(1,2,3-cd)pyrene	193-39-5
8	Benzal chloride	98-87-3	59	Isophorone	78-59-1
9	Benzamide	55-21-0	60	4,4'-Isopropylidenediphenol	80-05-7
10	Benzidine	92-87-5	61	Lindane	58-89-9
11	Benzo(a)anthracene	56-55-3	62	Maneb	12427-38-2
12	Benzo(b)fluoranthene	205-99-2	63	Melamine	108-78-1
13	Benzo(a)pyrene	50-32-8	64	Methoxychlor	72-43-5
14	Benzoic acid	65-85-0	65	4,4'-Methylenebis(2-chloroaniline)	101-14-4
15	Benzoic trichloride	98-07-7	66	4,4'-Methylenebis(N,N-dimethyl)benzenamine	101-61-1
16	Benzoyl chloride	98-88-4	67	4,4'-Methylenedianiline	101-77-9
17	Benzyl chloride	100-44-7	68	Michler's ketone	90-94-8
18	Bis(2-chloro-1-methylethyl)ether	108-60-1	69	N,N-Dimethylaniline	121-69-7
19	Bis(2-chloroethyl)ether	111-44-4	70	N-Nitrosodi-n-butylamine	924-16-3
20	Bromoheptane	629-04-9	71	N-Nitrosodi-n-propylamine	621-64-7
21	Captan	133-06-2	72	N-Nitrosodiphenylamine	86-30-6
22	Catechol	120-80-9	73	N-Nitrosomorpholine	59-89-2
23	Chloramben	133-90-4	74	N-Nitrosopiperidine	100-75-4
24	p-Chloro-m-cresol	59-50-7	75	a-Naphthylamine	134-32-7
25	2-Chloroacetophenone (Tear gas)	532-27-4	76	ß-Naphthylamine	91-59-8
26	Chlorobenzilate	510-15-6	77	5-Nitro-o-anisidine	99-59-2
27	Chlorothalonil	1897-45-6	78	Nitrobenzene	98-95-3
28	p-Cresidine	120-71-8	79	4-Nitrobiphenyl	92-93-3
29	m-Cresol	108-39-4	80	Nitrofen	1836-75-5
30	Cumene	98-82-8	81	2-Nitrophenol	88-75-5
31	Cumene hydroperoxide	80-15-9	82	4-Nitrophenol	100-02-7
32	2,4-D	94-75-7	83	Octachloronaphthalene	2234-13-1
33	Decabromodiphenyl oxide	1163-19-5	84	Parathion	56-38-2
34	2,4-Diaminoanisole	615-05-4	85	p-Phenylenediamine	106-50-3
35	4,4'-Diaminodiphenyl ether	101-80-4	86	Phthalic anhydride	85-44-9
36	Dibenz(a,h)anthracene	53-70-3	87	Picric acid	88-89-1
37	1,2-Dibromo-3-chloropropane	96-12-8	88	Propane sultone	1120-71-4
38	3,3'-Dichlorobenzidine	91-94-1	89	Propoxur	114-26-1
39	Dichlorvos	62-73-7	90	Quinoline	91-22-5
40	Dicofol	115-32-2	91	Quintozene (Pentachloronitrobenzene)	82-68-8
41	Diethyl sulfate	64-67-5	92	Styrene oxide	96-09-3
42	3,3'-Dimethoxybenzidine	119-90-4	93	Terephthalic acid	100-21-0
43	2,4-Dimethyl phenol	105-67-9	94	Tetrachlorvinphos	961-11-5
44	Dimethyl sulfate	77-78-1	95	4,4'-Thiodianiline	139-65-1
45	4-Dimethylaminoazobenzene	60-11-7	96	Toluene-2,4-diisocyanate	584-84-9
46	3,3'-Dimethylbenzidine	119-93-7	97	o-Toluidine	95-53-4
47	Dimethylcarbamyl chloride	79-44-7	98	o-Toluidine hydrochloride	636-21-5
48	4,6-Dinitro-o-cresol	534-52-1	99	Trifluralin	1582-09-8
49	2,4-Dinitrophenol	51-28-5	100	Tris(2,3-dibromopropyl) phosphate	126-72-7
50	2,4-Dinitrotoluene	121-14-2	101	Zineb	12122-67-7
51	2,6-Dinitrotoluene	606-20-2			

V. DISCUSSION

A. Limitations of the FY82 Data

Several limitations of the FY82 data files posed problems for this analysis. These limitations are the same as those described detail in the original unidentified peaks report (Onstot 1986a). In summary, most of the major problems revolved around the extremely complex sample matrix encountered in most of the samples, a mass scanning range used in the semivolatile analysis (m/z 100-700 amu) that was inappropriate for the proper identification of many compounds, and somewhat erratic retention times observed in the semivolatile composites which sometimes made identification of specific isomers difficult and unreliable.

The higher than normal mass scanning range was originally chosen to allow detection of polybrominated biphenyls and was thus appropriate for its intended purpose. Similarly, the erratic retention time values were not a problem in the broad scan study because standards were run daily and slight corrections could be made to the broad scan target compound RRTs. However, the lack of daily target analyte standards specific for the current study and associated retention information made RRT corrections slightly less reliable in this study. Corrections were primarily based on observed changes to the elution times of internal standards and surrogate compounds. This proved adequate for the volatiles which contained four standard compounds, and for the 6% semivolatiles, which contained seven standard compounds; but was marginally adequate for the 15/50% semivolatiles, which contained only one standard compound.

B. Retention Prediction

The relative retention time scheme proved generally successful, with most identified compounds having been observed well within the predicted retention window. However, the accuracy of prediction using this approach is known to be affected by a number of chemical and physical parameters. Interactions between the compounds of interest and the GC stationary phase can result in different retention characteristics between polar and nonpolar compounds. Thus, if the retention regression is based on a set of nonpolar compounds, predictions for polar compounds based on the nonpolar regression curve may be inaccurate (Kovats 1965). Interaction between sample components in the GC column can also influence elution times. This effect may sometimes be observed when a trace component is eluted on the back edge of a major component; the major component will take part in the separation process, thus acting as a "dynamic stationary phase" (Deans 1971). Since a large number of major components were present in the FY82 data, this phenomenon may have been responsible for some inaccuracies in observed retentions. Reproducibility of various GC operating conditions such as column temperature programming, carrier gas flow rate and injector temperature may also affect retention characteristics (Schomburg 1973 Ettre 1984). Changes in retentive properties of a column stationary phase may affect retention indices over time and are probably due to oxidiative degradation of the phase.

In spite of the limitations described above, prediction of retention values proved to generally successful for most compounds because the search window was set wide enough that minor errors in retention could be tolerated. The method was less successful in identifying closely eluting isomers with similar mass spectra, such as cumene and trimethylbenzene (C_9H_{12}).

C. Additional Problems Associated with VOA Analysis

The most persistent problem encountered during the TCA analysis of the VOA composites was associated with the nonspecificity of some target mass spectra, i.e., the mass spectra of many target compounds were not distinctive enough to distinguish them from the many large nontarget peaks observed throughout the chromatogram. A listing of compounds which were judged to have nonspecific mass spectra is shown in Table 15. It should be noted that nonspecificity is related not only to the mass spectrum itself but may also be associated with the sample matrix. As a result, trichloroethylene, which coeluted with the major constituent pentanal was relatively easy to positively identify because no interfering compounds with similar spectra were observed within its retention window. On the other hand, the presence of acetone was difficult to verify due the presence of a nontarget coeluting compound with common fragment ions and their mass spectra could not be separated by enhancement or subtraction routines. As a result, acetone was considered not detected although its presence is suggested in many of the composites.

D. Additional Problems Associated with SMV Analysis

Some compounds in the semivolatile target group were difficult to positively identify because of the nonspecificity of their mass spectra, similar to that described for the volatile target compounds. For the semivolatile analytes; however, this problem was exascerbated by the high mass scanning range, as described previously. For example, very little fragmentation was observable for the cresols because the mass spectrometer did not collect data below 100 amu, and as a result, only the molecular ion and M-1 ion (m/z 108 and 107) are visible in the mass spectrum. However, the M/M-1 ratio for cresol is relatively distinctive, and in some instances three responses corresponding to the cresol elution pattern were observed. These two factors led to the decision to report the identification of the cresol isomers. It should be emphasized, however, that the identification of cresols is based on extremely limited mass spectral information. Other semivolatile compounds which presented problems due to limited mass spectral specificity are shown in Table 16.

E. Comparison of Authentic Standards to Observed Targets

All of the compounds tentatively identified in the TCA analysis portion of this study were verified via GC/MS analysis of authentic standard material, with the exception of pentyl benzaldehyde, which could not be obtained in time for the authentic standard analysis portion of this study. The results of the authentic standard comparison are shown in Table 17.

Table 15
Volatile Compounds with Non-Specific Mass Spectra

Carbon Disulfide
Ethyleneimine (Aziridine)
1,2-Butylene oxide
Vinyl acetate
Acetonitrile
Methyl ethyl ketone
Isopropyl alcohol
Ethyl acrylate
Acrolein
Propylamineimine
t-Butyl alcohol
sec-Butanol
Ethyl acrylate
Nitropropane
Acrylic acid

Table 16
Semivolatile Compounds with Non-Specific Mass Spectra

Cumene
Dimethylcarbamyl chloride
1,2,4-Trimethyl benzene
Cymeme
Propane Sulfone
Bis(2-chloroethyl) ether
Dimethyl sulfate
Styrene oxide
Benzoyl chloride
o-Cresol
m-Cresol
p-Cresol
N-Nitrosomorpholine
Nitrobenzene
Isophorone
N-Nitrosopiperidine
o-Toluidine hydrochloride
Hydroquinone
Catechol
Phenylenediamine
Michler's ketone

Table 17

Comparison of Authentic Standards vs Observed Targets

Volatiles Compound Name	Average Observed RRT	Authentic Std. RRT	Δ RRT (%)	RRT Range Observed in Composites	Authentic RRf
Isobutyraldehyde	.332	.309	-7.4	.311 - .350	.070
Butyraldehyde	.372	.358	-3.9	.353 - .390	.040
Trichloroethene	.606	.639	5.2	.593 - .623	.335
1-Bromopentane	1.508	1.421	-6.1	1.494 - 1.529	.660
1-Pentanol	1.127	1.004	-12.3	1.067 - 1.205	.020
1-Nonene	1.911	1.933	1.1	1.820 - 2.084	.210
Ethyl isovalerate	1.705	1.628	-4.7	1.630 - 1.803	.315
1-Iodopentane	2.188	2.144	-2.1	2.066 - 2.376	.115
2-Pentyl furan	2.742	2.768	.9	2.573 - 3.012	.170
Limonene	2.966	3.060	3.1	2.771 - 3.269	.110
1-Bromoheptane	3.093	3.137	1.4	3.011 - 3.168	.220
Pentyl cyclohexane	3.532	3.642	3.0	3.403 - 3.908	.160
3-Octen-2-one	3.124	3.151	.9	2.876 - 3.824	.010

6% Semivolatiles Compound Name	Average Observed RRT	Authentic Std. Adjusted RRT	Δ RRT (%)	RRT Range Observed in Composites	Authentic RRf
Cumene	.267	.222	-20.3	.217 - .344	1.173
1,2,4-Trimethylbenzene	.292	.291	-.3	.247 - .323	1.220
Cymene	.321	.324	.9	.277 - .348	1.620
Limonene	.324	.328	1.2	.281 - .352	.150
2,6-Xylidene	.460	.468	1.7	.437 - .479	.811
Safrole	.582	.588	1.0	.572 - .593	.478
Biphenyl	.666	.671	.7	.656 - .674	1.286
Diphenyl ether	.686	.695	1.3	.671 - .781	.658
Dibenzofuran	.789	.791	.3	.786 - .793	1.272
Anthracene	1.002	1.002	.0	1.002 - 1.002	1.439

15/50% Semivolatiles Compound Name	Average Observed RRT	Authentic Std. Adjusted RRT	Δ RRT (%)	RRT Range Observed in Composites	Authentic RRf
o-Cresol	.347	.345	-.6	.291 - .398	.651
m-Cresol	.369	.367	-.5	.346 - .412	.638
p-Cresol	.380	.367	-3.5	.332 - .428	.638
2-Ethoxy benzaldehyde	.617	.600	-2.8	.611 - .623	.031
Diaminotoluene	.660	.673	1.9	.645 - .785	.581
2-Phenyl phenol	.784	.784	.0	.777 - .790	.333
Carbaryl	1.081	.776	-39.3	1.081 - 1.081	.212
Butyl phthalate butyl glycolate	1.330	1.304	-2.0	1.326 - 1.335	.053
Bis(2-ethylhexyl) adipate	1.371	1.347	-1.8	1.360 - 1.379	.733
Bis(2-ethylhexyl) phthalate	1.455	1.427	-2.0	1.442 - 1.465	.898

As can be seen in Table 17, most of the relative retention times of the authentic standards agree very well with the average RRT values of the tentatively identified compounds, with 23 compounds (out of a total of 33) having a percent relative difference of 3% or less.

One compound, *m*-cresol, was removed from the list of identified compounds because it was found to actually coelute with the para isomer (three distinct isomers of cresol were thought to have been observed in the actual samples). Since the actual identification of *p*- vs. *m*-cresol isomers could not be determined from the data, the identified peaks are referred to as "*m,p*-cresol" to signify that the peak could be either meta, para, or a combination of the two.

One compound, carbaryl, was found to elute much earlier than was observed in the original analysis. However, carbaryl was not removed from the list of identified compounds because the mass spectrum of carbaryl still showed a very high similarity to the spectrum observed in the composite.

One compound, cumene, was rejected because its actual RRT was significantly different from the tentatively identified peak RRT. However, unlike carbaryl, the mass spectral similarity of cumene to the respective tentatively identified peaks was not a sufficiently compelling reason to retain it on the list of identified compounds.

Several compounds were retained on the list of identified compounds even though the RRT of the authentic standards did not fall within the range of their respective tentatively identified peaks. In these cases, the discrepancy is suspected to be caused by differences between the two analyses which could not be entirely eliminated through normalization. In all these cases, the high similarity of the reference mass spectra to the tentatively identified peak mass spectra was a critical factor.

One compound was actually added to the list of identified compounds as a result of the authentic standards analysis. Diphenyl ether was added to the list when it was found that it bore a close resemblance to the mass spectra originally assigned to 2-phenyl phenol in the 6% semivolatile fraction. These two compounds both have the same empirical formula, $C_{12}H_{10}O$, and very similar mass spectra. However, the RRTs of the peaks in the 6% fraction were significantly different from those in the 15/50% fraction samples, even though both analyses were performed using the same GC conditions. The identification of diphenyl ether was confirmed using an authentic standard for comparison.

Positively identified compounds were quantitated in the adipose composites using the response factors generated from the authentic standards analysis. The quantitative results for each of the positively identified compounds are presented in Appendices A through C. However, these results should only be regarded as estimates, since the response factors may difer significantly from what they might have been at the time of the original analysis.

F. Comparison of Frequency of Occurrence Results to Unidentified Peaks Study

The 16 ECAD compounds selected from the original peaks study for analysis were also identified in this study. However, the frequencies of occurrence that were observed in this study usually differed somewhat from those in the original study. These differences are due to the manner in which the peaks were selected for identification in the unidentified peaks study and to the inherent difference in selectivity between the two identification methods. In the original study, only peaks which were distinguishable from the total ion current baseline and which were reasonably separated from coeluting peaks were selected for analysis. By using the TCA procedure in this study, it was possible to identify compounds buried under high background and coeluting peaks, which resulted in a higher number of identifications of ECAD compounds than was observed in the original study. This difference is illustrated in Table 18, which presents the frequencies of occurrence for ECAD compounds from both the unidentified peaks study and the current study. In fact, there were no cases where the TCA procedure failed to identify as many occurrences of a compound as the unidentified peaks procedure, with the exception of hexene, which was not identified in the current task although it was tentatively identified in the original unidentified peaks study. Examination of the boiling point vs. retention time data from the original identification indicated that the peak originally identified as hexene eluted much later than would be expected and was probably an isomer of nonene.

Nonene itself was difficult to positively identify because several peaks were often observed with mass spectra that were highly similar to the nonene reference spectrum. These multiple peaks were assumed to be isomers of the general formula C_9H_{18}. In these circumstances, peak areas for all peaks passing the minimum FIT threshold were integrated and reported as "Nonenes." If the hexene and nonene frequencies of occurrence from the original unidentified peaks study are summed, the comparison of the frequency of nonenes in that study to the current study becomes 47/46.

G. Possible Sources of Identified Compounds

A preliminary search to determine possible sources of the identified compounds was conducted. All of the information below was found in the *Merck Index*, 10th edition, unless otherwise noted.

Table 18

Frequency of Occurrence of ECAD Analytes
In Original Unidentified Peaks Study and Current Study

Volatiles

No.	Compound Name	Freq. of Occurrence Unidentified Peaks	Freq. of Occurrence TCA Analysis
1	2-Amyl furan	29	46
2	Bromoheptane	2	4
3	Bromopentane	3	3
4	Ethyl isovalerate	16	44
5	Hexene	39	0
6	3-Octen-2-one	9	46
7	Limonene	44	46
8	Nonene	8	46
9	Pentyl alcohol	29	38
10	Pentyl cyclohexane	1	10

Semivolatiles

No.	Compound Name	Freq. of Occurrence Unidentified Peaks (a)	Freq. of Occurrence TCA Analysis (a)
1	Butyl glycol butyl phthalate	6\0	0\8
2	Cymene	7\0	41\0
3	2-Ethoxy benzaldehyde	0\4	0\6
4	4-Pentyl benzaldehyde	0\1	0\9
5	o-Phenyl Phenol (b)	0\18	0\22
6	Diphenyl ether (c)	35\0	40\0

Notes:

a. Frequencies of occurrence are shown for 6% and 15/50% Florisil fractions, respectively.
b. Identified as [1,1'-Biphenyl]-2-ol in Unidentified Peaks Study (Onstot, 1987).
c. Identified as 1,1'-Oxybis-benzene in Unidentified Peaks Study (Onstot, 1987).

Volatiles

Ethyl isovalerate	Used in alcoholic solution for flavoring confectionary and beverages.
Limonene	Found in various ethereal oils, particularly oils of lemon and orange. Lemon-like odor. Used as a solvent in the manufacture of resins, and as a wetting and dispersing agent.
Pentyl alcohol	Solvent.
Trichloroethylene	Solvent for fats, waxes, resins, etc. Used for solvent extraction in many industries. Also used as a degreasing agent in dry cleaning.

Semivolatiles

Anthracene	Combustion product; found in fossil fuels. Used as an intermediate in production of dyes (IARC Monograph).
Biphenyl	Used as a heat transfer agent, fungistat for oranges (applied to inside of shipping container or wrappers).
Diphenyl ether	Used as a heat transfer medium and in perfuming soaps.
Limonene	See volatiles.
2-Phenyl phenol	Dowicide 1; used as germicide and fungicide. Active ingredient in Lysol. This compound is suspected to be a contaminant from the adipose collection procedure.
Safrole	Topical antiseptic; used in the manufacture of heliotropin. Listed as EPA carcinogen.
Xylidene	Used in the manufacture of dyes.
Bis(ethylhexyl) phthalate	Plasticizer, vacuum pump oil.
Carbaryl	Contact insecticide.
Cresol	Used as local antiseptic, parasiticide, disinfectant, in photographic developing solutions, in manufacture of explosives.

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APPENDIX A

VOLATILE COMPOSITE SUMMARY REPORTS

Appendix A-1

FY82 VOA Adipose Composite Summary

CAS No.: 3777-69-3

Data Report - 2-Amyl furan

Fraction: VOA

RRf: 0.170

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	2.811	92.416	6.161	6/19/84
82-302	1 - PA - VO - 15-44	17.4	2.712	32.468	1.865	6/20/84
82-303	1 - PA - VO - 45+	20.7	2.699	33.199	1.603	6/20/84
82-304	1 - NE - VO - 0-14	20.0	2.684	246.867	12.343	6/20/84
82-305	1 - NE - VO - 15-44	23.6	2.667	571.778	24.227	6/21/84
82-306	1 - NE - VO - 45+	25.5	2.650	786.271	30.834	6/26/84
82-307	1 - MA - VO - 0-14	20.3	2.780	47.423	2.336	6/27/84
82-308	1 - MA - VO - 15-44	25.0	2.752	190.777	7.631	6/27/84
82-309	1 - MA - VO - 45+	15.5	2.774	153.481	9.902	6/27/84
82-310	1 - EN - VO - 0-14	12.7	2.785	94.927	7.474	6/28/84
82-311	1 - EN - VO - 15-44	20.8	2.714	73.326	3.525	6/28/84
82-312	1 - EN - VO - 45+	18.6	2.632	37.386	2.010	6/28/84
82-313	1 - WN - VO - 0-14	18.9	2.789	261.608	13.841	6/29/84
82-314	1 - WN - VO - 15-44	21.6	2.716	9.084	.420	6/29/84
82-315	1 - WN - VO - 45+	21.6	2.722	3.219	.149	7/2/84
82-316	1 - SA - VO - 0-14	12.6	2.837	564.965	44.838	7/3/84
82-317	1 - SA - VO - 15-44	22.2	2.937	42.548	1.916	7/3/84
82-318	1 - SA - VO - 45+	15.4	2.893	52.164	3.387	7/3/84
82-319	1 - ES - VO - 0-14	25.6	2.772	71.659	2.799	7/9/84
82-320	1 - ES - VO - 15-44	19.0	2.905	62.282	3.278	7/9/84
82-321	1 - ES - VO - 45+	20.6	2.859	98.328	4.773	7/9/84
82-322	1 - WS - VO - 0-14	6.0	2.844	264.880	44.146	7/11/84
82-323	1 - WS - VO - 15-44	22.4	2.724	480.778	21.463	7/11/84
82-324	1 - WS - VO - 45+	22.0	2.738	255.697	11.622	7/11/84
82-325	1 - MO - VO - 0-14	5.1	2.910	68.353	13.402	7/11/84
82-326	1 - MO - VO - 15-44	18.8	2.824	176.056	9.364	7/12/84
82-327	1 - MO - VO - 45+	22.4	2.987	328.794	14.678	7/12/84
82-328	2 - MA - VO - 0-14	18.1	2.835	98.021	5.415	7/12/84
82-329	2 - MA - VO - 15-44	25.3	2.866	183.018	7.233	7/13/84
82-330	2 - MA - VO - 45+	17.8	3.012	178.199	10.011	7/13/84
82-331	2 - EN - VO - 0-14	17.3	2.751	72.512	4.191	7/13/84
82-332	2 - EN - VO - 15-44	21.1	2.604	33.620	1.593	7/16/84
82-333	2 - EN - VO - 45+	22.6	ND	ND	ND	7/16/84
82-334	2 - WN - VO - 45+	18.3	2.664	9.482	.518	7/16/84
82-335	2 - SA - VO - 0-14	16.7	2.573	426.676	25.549	7/17/84
82-336	2 - SA - VO - 15-44	18.7	2.628	167.508	8.957	7/17/84
82-337	2 - SA - VO - 45+	23.2	2.650	30.274	1.304	7/17/84
82-338	2 - ES - VO - 15-44	24.3	2.600	14.449	.594	7/18/84
82-339	2 - ES - VO - 45+	19.3	2.636	64.277	3.330	7/20/84
82-340	2 - WS - VO - 15-44	21.9	2.592	74.050	3.381	7/18/84
82-341	3 - EN - VO - 15-44	19.6	2.582	18.030	.919	7/18/84
82-342	3 - EN - VO - 45+	21.4	2.598	64.955	3.035	7/18/84
82-343	3 - SA - VO - 15-44	10.1	2.649	83.036	8.221	7/20/84
82-344	3 - SA - VO - 45+	13.8	2.698	73.627	5.335	7/20/84
82-345	4 - SA - VO - 15-44	17.8	2.642	95.552	5.368	7/20/84
82-346	4 - SA - VO - 45+	11.6	2.720	25.318	2.182	7/20/84

Appendix A-2

FY82 VOA Adipose Composite Summary

CAS No.: 629-04-9

Data Report - Bromoheptane

Fraction: VOA

RRf: 0.220

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	3.117	.247	.016	6/19/84
82-302	1 - PA - VO - 15-44	17.4	ND	ND	ND	6/20/84
82-303	1 - PA - VO - 45+	20.7	ND	ND	ND	6/20/84
82-304	1 - NE - VO - 0-14	20.0	ND	ND	ND	6/20/84
82-305	1 - NE - VO - 15-44	23.6	ND	ND	ND	6/21/84
82-306	1 - NE - VO - 45+	25.5	ND	ND	ND	6/26/84
82-307	1 - MA - VO - 0-14	20.3	ND	ND	ND	6/27/84
82-308	1 - MA - VO - 15-44	25.0	ND	ND	ND	6/27/84
82-309	1 - MA - VO - 45+	15.5	ND	ND	ND	6/27/84
82-310	1 - EN - VO - 0-14	12.7	ND	ND	ND	6/28/84
82-311	1 - EN - VO - 15-44	20.8	ND	ND	ND	6/28/84
82-312	1 - EN - VO - 45+	18.6	ND	ND	ND	6/28/84
82-313	1 - WN - VO - 0-14	18.9	3.074	2.256	.119	6/29/84
82-314	1 - WN - VO - 15-44	21.6	ND	ND	ND	6/29/84
82-315	1 - WN - VO - 45+	21.6	ND	ND	ND	7/2/84
82-316	1 - SA - VO - 0-14	12.6	ND	ND	ND	7/3/84
82-317	1 - SA - VO - 15-44	22.2	ND	ND	ND	7/3/84
82-318	1 - SA - VO - 45+	15.4	ND	ND	ND	7/3/84
82-319	1 - ES - VO - 0-14	25.6	ND	ND	ND	7/9/84
82-320	1 - ES - VO - 15-44	19.0	ND	ND	ND	7/9/84
82-321	1 - ES - VO - 45+	20.6	3.168	.378	.018	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	3.011	1.553	.069	7/11/84
82-324	1 - WS - VO - 45+	22.0	ND	ND	ND	7/11/84
82-325	1 - MO - VO - 0-14	5.1	ND	ND	ND	7/11/84
82-326	1 - MO - VO - 15-44	18.8	ND	ND	ND	7/12/84
82-327	1 - MO - VO - 45+	22.4	ND	ND	ND	7/12/84
82-328	2 - MA - VO - 0-14	18.1	ND	ND	ND	7/12/84
82-329	2 - MA - VO - 15-44	25.3	ND	ND	ND	7/13/84
82-330	2 - MA - VO - 45+	17.8	ND	ND	ND	7/13/84
82-331	2 - EN - VO - 0-14	17.3	ND	ND	ND	7/13/84
82-332	2 - EN - VO - 15-44	21.1	ND	ND	ND	7/16/84
82-333	2 - EN - VO - 45+	22.6	ND	ND	ND	7/16/84
82-334	2 - WN - VO - 45+	18.3	ND	ND	ND	7/16/84
82-335	2 - SA - VO - 0-14	16.7	ND	ND	ND	7/17/84
82-336	2 - SA - VO - 15-44	18.7	ND	ND	ND	7/17/84
82-337	2 - SA - VO - 45+	23.2	ND	ND	ND	7/17/84
82-338	2 - ES - VO - 15-44	24.3	ND	ND	ND	7/18/84
82-339	2 - ES - VO - 45+	19.3	ND	ND	ND	7/20/84
82-340	2 - WS - VO - 15-44	21.9	ND	ND	ND	7/18/84
82-341	3 - EN - VO - 15-44	19.6	ND	ND	ND	7/18/84
82-342	3 - EN - VO - 45+	21.4	ND	ND	ND	7/18/84
82-343	3 - SA - VO - 15-44	10.1	ND	ND	ND	7/20/84
82-344	3 - SA - VO - 45+	13.8	ND	ND	ND	7/20/84
82-345	4 - SA - VO - 15-44	17.8	ND	ND	ND	7/20/84
82-346	4 - SA - VO - 45+	11.6	ND	ND	ND	7/20/84

Appendix A-3

FY82 VOA Adipose Composite Summary

CAS No.: 110-53-2

Data Report - Bromopentane

Fraction: VOA

RRf: 0.660

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	1.529	.021	.001	6/19/84
82-302	1 - PA - VO - 15-44	17.4	ND	ND	ND	6/20/84
82-303	1 - PA - VO - 45+	20.7	ND	ND	ND	6/20/84
82-304	1 - NE - VO - 0-14	20.0	ND	ND	ND	6/20/84
82-305	1 - NE - VO - 15-44	23.6	ND	ND	ND	6/21/84
82-306	1 - NE - VO - 45+	25.5	ND	ND	ND	6/26/84
82-307	1 - MA - VO - 0-14	20.3	ND	ND	ND	6/27/84
82-308	1 - MA - VO - 15-44	25.0	ND	ND	ND	6/27/84
82-309	1 - MA - VO - 45+	15.5	ND	ND	ND	6/27/84
82-310	1 - EN - VO - 0-14	12.7	ND	ND	ND	6/28/84
82-311	1 - EN - VO - 15-44	20.8	ND	ND	ND	6/28/84
82-312	1 - EN - VO - 45+	18.6	ND	ND	ND	6/28/84
82-313	1 - WN - VO - 0-14	18.9	1.500	.072	.003	6/29/84
82-314	1 - WN - VO - 15-44	21.6	ND	ND	ND	6/29/84
82-315	1 - WN - VO - 45+	21.6	ND	ND	ND	7/2/84
82-316	1 - SA - VO - 0-14	12.6	ND	ND	ND	7/3/84
82-317	1 - SA - VO - 15-44	22.2	ND	ND	ND	7/3/84
82-318	1 - SA - VO - 45+	15.4	ND	ND	ND	7/3/84
82-319	1 - ES - VO - 0-14	25.6	ND	ND	ND	7/9/84
82-320	1 - ES - VO - 15-44	19.0	ND	ND	ND	7/9/84
82-321	1 - ES - VO - 45+	20.6	ND	ND	ND	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	1.494	.031	.001	7/11/84
82-324	1 - WS - VO - 45+	22.0	ND	ND	ND	7/11/84
82-325	1 - MO - VO - 0-14	5.1	ND	ND	ND	7/11/84
82-326	1 - MO - VO - 15-44	18.8	ND	ND	ND	7/12/84
82-327	1 - MO - VO - 45+	22.4	ND	ND	ND	7/12/84
82-328	2 - MA - VO - 0-14	18.1	ND	ND	ND	7/12/84
82-329	2 - MA - VO - 15-44	25.3	ND	ND	ND	7/13/84
82-330	2 - MA - VO - 45+	17.8	ND	ND	ND	7/13/84
82-331	2 - EN - VO - 0-14	17.3	ND	ND	ND	7/13/84
82-332	2 - EN - VO - 15-44	21.1	ND	ND	ND	7/16/84
82-333	2 - EN - VO - 45+	22.6	ND	ND	ND	7/16/84
82-334	2 - WN - VO - 45+	18.3	ND	ND	ND	7/16/84
82-335	2 - SA - VO - 0-14	16.7	ND	ND	ND	7/17/84
82-336	2 - SA - VO - 15-44	18.7	ND	ND	ND	7/17/84
82-337	2 - SA - VO - 45+	23.2	ND	ND	ND	7/17/84
82-338	2 - ES - VO - 15-44	24.3	ND	ND	ND	7/18/84
82-339	2 - ES - VO - 45+	19.3	ND	ND	ND	7/20/84
82-340	2 - WS - VO - 15-44	21.9	ND	ND	ND	7/18/84
82-341	3 - EN - VO - 15-44	19.6	ND	ND	ND	7/18/84
82-342	3 - EN - VO - 45+	21.4	ND	ND	ND	7/18/84
82-343	3 - SA - VO - 15-44	10.1	ND	ND	ND	7/20/84
82-344	3 - SA - VO - 45+	13.8	ND	ND	ND	7/20/84
82-345	4 - SA - VO - 15-44	17.8	ND	ND	ND	7/20/84
82-346	4 - SA - VO - 45+	11.6	ND	ND	ND	7/20/84

Appendix A-4

FY82 VOA Adipose Composite Summary

CAS No.: 123-72-8

Data Report - Butyraldehyde

Fraction: VOA

RRf: 0.040

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	.372	14.785	.985	6/19/84
82-302	1 - PA - VO - 15-44	17.4	.367	42.384	2.435	6/20/84
82-303	1 - PA - VO - 45+	20.7	.372	12.620	.609	6/20/84
82-304	1 - NE - VO - 0-14	20.0	.360	62.288	3.114	6/20/84
82-305	1 - NE - VO - 15-44	23.6	.361	34.594	1.465	6/21/84
82-306	1 - NE - VO - 45+	25.5	.356	184.550	7.237	6/26/84
82-307	1 - MA - VO - 0-14	20.3	.372	17.077	.841	6/27/84
82-308	1 - MA - VO - 15-44	25.0	.366	35.145	1.405	6/27/84
82-309	1 - MA - VO - 45+	15.5	.365	21.672	1.398	6/27/84
82-310	1 - EN - VO - 0-14	12.7	.378	24.404	1.921	6/28/84
82-311	1 - EN - VO - 15-44	20.8	.353	31.908	1.534	6/28/84
82-312	1 - EN - VO - 45+	18.6	.363	28.191	1.515	6/28/84
82-313	1 - WN - VO - 0-14	18.9	.367	12.477	.660	6/29/84
82-314	1 - WN - VO - 15-44	21.6	.375	48.676	2.253	6/29/84
82-315	1 - WN - VO - 45+	21.6	.378	14.990	.693	7/2/84
82-316	1 - SA - VO - 0-14	12.6	.369	47.197	3.745	7/3/84
82-317	1 - SA - VO - 15-44	22.2	.390	23.713	1.068	7/3/84
82-318	1 - SA - VO - 45+	15.4	.383	13.047	.847	7/3/84
82-319	1 - ES - VO - 0-14	25.6	.372	36.927	1.442	7/9/84
82-320	1 - ES - VO - 15-44	19.0	.382	15.982	.841	7/9/84
82-321	1 - ES - VO - 45+	20.6	.385	35.807	1.738	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	.360	139.731	6.238	7/11/84
82-324	1 - WS - VO - 45+	22.0	.365	71.595	3.254	7/11/84
82-325	1 - MO - VO - 0-14	5.1	.384	4.257	.834	7/11/84
82-326	1 - MO - VO - 15-44	18.8	.374	21.889	1.164	7/12/84
82-327	1 - MO - VO - 45+	22.4	.388	34.830	1.554	7/12/84
82-328	2 - MA - VO - 0-14	18.1	.377	20.272	1.120	7/12/84
82-329	2 - MA - VO - 15-44	25.3	.380	25.477	1.007	7/13/84
82-330	2 - MA - VO - 45+	17.8	.388	20.999	1.179	7/13/84
82-331	2 - EN - VO - 0-14	17.3	.364	39.694	2.294	7/13/84
82-332	2 - EN - VO - 15-44	21.1	.366	47.979	2.273	7/16/84
82-333	2 - EN - VO - 45+	22.6	.369	23.045	1.019	7/16/84
82-334	2 - WN - VO - 45+	18.3	.380	20.570	1.124	7/16/84
82-335	2 - SA - VO - 0-14	16.7	.359	75.867	4.542	7/17/84
82-336	2 - SA - VO - 15-44	18.7	.368	77.784	4.159	7/17/84
82-337	2 - SA - VO - 45+	23.2	.367	67.073	2.891	7/17/84
82-338	2 - ES - VO - 15-44	24.3	.366	16.633	.684	7/18/84
82-339	2 - ES - VO - 45+	19.3	.370	14.297	.740	7/20/84
82-340	2 - WS - VO - 15-44	21.9	.367	24.659	1.125	7/18/84
82-341	3 - EN - VO - 15-44	19.6	.367	21.165	1.079	7/18/84
82-342	3 - EN - VO - 45+	21.4	.369	18.583	.868	7/18/84
82-343	3 - SA - VO - 15-44	10.1	.372	25.306	2.505	7/20/84
82-344	3 - SA - VO - 45+	13.8	.375	22.985	1.665	7/20/84
82-345	4 - SA - VO - 15-44	17.8	.372	38.072	2.138	7/20/84
82-346	4 - SA - VO - 45+	11.6	.384	32.029	2.761	7/20/84

Appendix A-5

FY82 VOA Adipose Composite Summary

CAS No.: 108-64-

Data Report - Ethyl isovalerate

Fraction: VO

RRf: 0.31

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	1.756	4.177	.278	6/19/84
82-302	1 - PA - VO - 15-44	17.4	1.719	6.959	.399	6/20/84
82-303	1 - PA - VO - 45+	20.7	1.710	8.590	.414	6/20/84
82-304	1 - NE - VO - 0-14	20.0	1.702	18.173	.908	6/20/84
82-305	1 - NE - VO - 15-44	23.6	1.690	7.618	.322	6/21/84
82-306	1 - NE - VO - 45+	25.5	1.691	2.419	.094	6/26/84
82-307	1 - MA - VO - 0-14	20.3	1.721	.554	.027	6/27/84
82-308	1 - MA - VO - 15-44	25.0	1.702	6.432	.257	6/27/84
82-309	1 - MA - VO - 45+	15.5	1.715	3.227	.208	6/27/84
82-310	1 - EN - VO - 0-14	12.7	1.722	33.380	2.628	6/28/84
82-311	1 - EN - VO - 15-44	20.8	1.718	53.504	2.572	6/28/84
82-312	1 - EN - VO - 45+	18.6	1.683	15.441	.830	6/28/84
82-313	1 - WN - VO - 0-14	18.9	1.718	5.497	.290	6/29/84
82-314	1 - WN - VO - 15-44	21.6	1.701	8.572	.396	6/29/84
82-315	1 - WN - VO - 45+	21.6	1.702	6.998	.324	7/2/84
82-316	1 - SA - VO - 0-14	12.6	1.734	.341	.027	7/3/84
82-317	1 - SA - VO - 15-44	22.2	1.775	13.665	.615	7/3/84
82-318	1 - SA - VO - 45+	15.4	1.759	15.850	1.029	7/3/84
82-319	1 - ES - VO - 0-14	25.6	1.725	.918	.035	7/9/84
82-320	1 - ES - VO - 15-44	19.0	1.769	13.562	.713	7/9/84
82-321	1 - ES - VO - 45+	20.6	ND	ND	ND	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	1.697	35.999	1.607	7/11/84
82-324	1 - WS - VO - 45+	22.0	1.703	34.945	1.588	7/11/84
82-325	1 - MO - VO - 0-14	5.1	1.753	.190	.037	7/11/84
82-326	1 - MO - VO - 15-44	18.8	1.729	2.752	.146	7/12/84
82-327	1 - MO - VO - 45+	22.4	1.789	11.199	.499	7/12/84
82-328	2 - MA - VO - 0-14	18.1	1.738	2.832	.156	7/12/84
82-329	2 - MA - VO - 15-44	25.3	1.753	.397	.015	7/13/84
82-330	2 - MA - VO - 45+	17.8	1.803	4.105	.230	7/13/84
82-331	2 - EN - VO - 0-14	17.3	1.705	8.890	.513	7/13/84
82-332	2 - EN - VO - 15-44	21.1	1.654	4.434	.210	7/16/84
82-333	2 - EN - VO - 45+	22.6	1.652	7.117	.314	7/16/84
82-334	2 - WN - VO - 45+	18.3	1.682	5.371	.293	7/16/84
82-335	2 - SA - VO - 0-14	16.7	1.630	1.175	.070	7/17/84
82-336	2 - SA - VO - 15-44	18.7	1.660	39.797	2.128	7/17/84
82-337	2 - SA - VO - 45+	23.2	1.669	10.221	.440	7/17/84
82-338	2 - ES - VO - 15-44	24.3	1.654	1.828	.075	7/18/84
82-339	2 - ES - VO - 45+	19.3	1.665	7.430	.385	7/20/84
82-340	2 - WS - VO - 15-44	21.9	1.650	31.811	1.452	7/18/84
82-341	3 - EN - VO - 15-44	19.6	1.646	18.212	.929	7/18/84
82-342	3 - EN - VO - 45+	21.4	1.652	14.874	.695	7/18/84
82-343	3 - SA - VO - 15-44	10.1	1.667	12.585	1.246	7/20/84
82-344	3 - SA - VO - 45+	13.8	1.684	7.178	.520	7/20/84
82-345	4 - SA - VO - 15-44	17.8	1.667	6.470	.363	7/20/84
82-346	4 - SA - VO - 45+	11.6	1.713	11.502	.991	7/20/84

Appendix A-6

FY82 VOA Adipose Composite Summary

CAS No.: 628-17-1

Data Report - 1-Iodopentane

Fraction: VOA

RRf: 0.115

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	2.250	.996	.066	6/19/84
82-302	1 - PA - VO - 15-44	17.4	2.189	.246	.014	6/20/84
82-303	1 - PA - VO - 45+	20.7	2.176	.871	.042	6/20/84
82-304	1 - NE - VO - 0-14	20.0	2.167	.328	.016	6/20/84
82-305	1 - NE - VO - 15-44	23.6	2.143	4.147	.175	6/21/84
82-306	1 - NE - VO - 45+	25.5	2.139	26.769	1.049	6/26/84
82-307	1 - MA - VO - 0-14	20.3	ND	ND	ND	6/27/84
82-308	1 - MA - VO - 15-44	25.0	2.200	.674	.026	6/27/84
82-309	1 - MA - VO - 45+	15.5	2.217	.436	.028	6/27/84
82-310	1 - EN - VO - 0-14	12.7	2.218	.131	.010	6/28/84
82-311	1 - EN - VO - 15-44	20.8	ND	ND	ND	6/28/84
82-312	1 - EN - VO - 45+	18.6	ND	ND	ND	6/28/84
82-313	1 - WN - VO - 0-14	18.9	2.218	1.094	.057	6/29/84
82-314	1 - WN - VO - 15-44	21.6	2.183	.194	.008	6/29/84
82-315	1 - WN - VO - 45+	21.6	2.181	.186	.008	7/2/84
82-316	1 - SA - VO - 0-14	12.6	ND	ND	ND	7/3/84
82-317	1 - SA - VO - 15-44	22.2	ND	ND	ND	7/3/84
82-318	1 - SA - VO - 45+	15.4	2.297	.153	.009	7/3/84
82-319	1 - ES - VO - 0-14	25.6	2.223	.258	.010	7/9/84
82-320	1 - ES - VO - 15-44	19.0	ND	ND	ND	7/9/84
82-321	1 - ES - VO - 45+	20.6	2.285	.643	.031	7/9/84
82-322	1 - WS - VO - 0-14	6.0	2.272	1.292	.215	7/11/84
82-323	1 - WS - VO - 15-44	22.4	2.172	.894	.039	7/11/84
82-324	1 - WS - VO - 45+	22.0	2.188	1.532	.069	7/11/84
82-325	1 - MO - VO - 0-14	5.1	2.283	.510	.100	7/11/84
82-326	1 - MO - VO - 15-44	18.8	2.250	3.220	.171	7/12/84
82-327	1 - MO - VO - 45+	22.4	ND	ND	ND	7/12/84
82-328	2 - MA - VO - 0-14	18.1	ND	ND	ND	7/12/84
82-329	2 - MA - VO - 15-44	25.3	2.283	.477	.018	7/13/84
82-330	2 - MA - VO - 45+	17.8	2.376	.420	.023	7/13/84
82-331	2 - EN - VO - 0-14	17.3	2.193	.120	.006	7/13/84
82-332	2 - EN - VO - 15-44	21.1	2.107	.643	.030	7/16/84
82-333	2 - EN - VO - 45+	22.6	ND	ND	ND	7/16/84
82-334	2 - WN - VO - 45+	18.3	2.147	.090	.004	7/16/84
82-335	2 - SA - VO - 0-14	16.7	2.066	.355	.021	7/17/84
82-336	2 - SA - VO - 15-44	18.7	2.115	.803	.042	7/17/84
82-337	2 - SA - VO - 45+	23.2	2.127	.159	.006	7/17/84
82-338	2 - ES - VO - 15-44	24.3	2.107	1.108	.045	7/18/84
82-339	2 - ES - VO - 45+	19.3	2.127	.470	.024	7/20/84
82-340	2 - WS - VO - 15-44	21.9	2.092	.535	.024	7/18/84
82-341	3 - EN - VO - 15-44	19.6	2.089	.171	.008	7/18/84
82-342	3 - EN - VO - 45+	21.4	ND	ND	ND	7/18/84
82-343	3 - SA - VO - 15-44	10.1	2.127	.972	.096	7/20/84
82-344	3 - SA - VO - 45+	13.8	ND	ND	ND	7/20/84
82-345	4 - SA - VO - 15-44	17.8	ND	ND	ND	7/20/84
82-346	4 - SA - VO - 45+	11.6	2.192	.568	.048	7/20/84

Appendix A-7

FY82 VOA Adipose Composite Summary

CAS No.: 78-84-2

Data Report - Isobutyraldehyde

Fraction: VOA

RRf: 0.070

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	.333	1.441	.096	6/19/84
82-302	1 - PA - VO - 15-44	17.4	.325	4.136	.237	6/20/84
82-303	1 - PA - VO - 45+	20.7	.338	.153	.007	6/20/84
82-304	1 - NE - VO - 0-14	20.0	.323	5.088	.254	6/20/84
82-305	1 - NE - VO - 15-44	23.6	.324	2.277	.096	6/21/84
82-306	1 - NE - VO - 45+	25.5	.319	17.770	.696	6/26/84
82-307	1 - MA - VO - 0-14	20.3	.333	5.503	.271	6/27/84
82-308	1 - MA - VO - 15-44	25.0	.328	6.358	.254	6/27/84
82-309	1 - MA - VO - 45+	15.5	.326	4.285	.276	6/27/84
82-310	1 - EN - VO - 0-14	12.7	.332	1.350	.106	6/28/84
82-311	1 - EN - VO - 15-44	20.8	.311	7.107	.341	6/28/84
82-312	1 - EN - VO - 45+	18.6	.319	1.908	.102	6/28/84
82-313	1 - WN - VO - 0-14	18.9	.328	1.918	.101	6/29/84
82-314	1 - WN - VO - 15-44	21.6	.329	2.104	.097	6/29/84
82-315	1 - WN - VO - 45+	21.6	.335	1.542	.071	7/2/84
82-316	1 - SA - VO - 0-14	12.6	.333	2.877	.228	7/3/84
82-317	1 - SA - VO - 15-44	22.2	.348	2.138	.096	7/3/84
82-318	1 - SA - VO - 45+	15.4	.342	1.843	.119	7/3/84
82-319	1 - ES - VO - 0-14	25.6	.333	3.362	.131	7/9/84
82-320	1 - ES - VO - 15-44	19.0	ND	ND	ND	7/9/84
82-321	1 - ES - VO - 45+	20.6	.341	1.956	.094	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	.318	8.935	.398	7/11/84
82-324	1 - WS - VO - 45+	22.0	.326	5.447	.247	7/11/84
82-325	1 - MO - VO - 0-14	5.1	.344	.484	.094	7/11/84
82-326	1 - MO - VO - 15-44	18.8	.334	4.093	.217	7/12/84
82-327	1 - MO - VO - 45+	22.4	.350	3.759	.167	7/12/84
82-328	2 - MA - VO - 0-14	18.1	.337	4.476	.247	7/12/84
82-329	2 - MA - VO - 15-44	25.3	.340	3.589	.141	7/13/84
82-330	2 - MA - VO - 45+	17.8	.350	2.905	.163	7/13/84
82-331	2 - EN - VO - 0-14	17.3	.325	2.351	.135	7/13/84
82-332	2 - EN - VO - 15-44	21.1	.327	4.691	.222	7/16/84
82-333	2 - EN - VO - 45+	22.6	.329	2.303	.101	7/16/84
82-334	2 - WN - VO - 45+	18.3	.339	2.396	.130	7/16/84
82-335	2 - SA - VO - 0-14	16.7	.320	3.127	.187	7/17/84
82-336	2 - SA - VO - 15-44	18.7	.328	4.241	.226	7/17/84
82-337	2 - SA - VO - 45+	23.2	ND	ND	ND	7/17/84
82-338	2 - ES - VO - 15-44	24.3	.327	3.578	.147	7/18/84
82-339	2 - ES - VO - 45+	19.3	.334	3.044	.157	7/20/84
82-340	2 - WS - VO - 15-44	21.9	.328	2.536	.115	7/18/84
82-341	3 - EN - VO - 15-44	19.6	.328	2.214	.112	7/18/84
82-342	3 - EN - VO - 45+	21.4	.329	1.534	.071	7/18/84
82-343	3 - SA - VO - 15-44	10.1	.332	5.021	.497	7/20/84
82-344	3 - SA - VO - 45+	13.8	.338	3.124	.226	7/20/84
82-345	4 - SA - VO - 15-44	17.8	.332	2.340	.131	7/20/84
82-346	4 - SA - VO - 45+	11.6	.343	2.042	.176	7/20/84

Appendix A-8

FY82 VOA Adipose Composite Summary

CAS No.: 138-86-3

Data Report - Limonene

Fraction: VOA

RRf: 0.110

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	3.047	57.455	3.830	6/19/84
82-302	1 - PA - VO - 15-44	17.4	2.931	5.285	.303	6/20/84
82-303	1 - PA - VO - 45+	20.7	2.921	17.318	.836	6/20/84
82-304	1 - NE - VO - 0-14	20.0	2.903	2.140	.107	6/20/84
82-305	1 - NE - VO - 15-44	23.6	2.874	15.899	.673	6/21/84
82-306	1 - NE - VO - 45+	25.5	2.856	20.240	.793	6/26/84
82-307	1 - MA - VO - 0-14	20.3	3.011	1.659	.081	6/27/84
82-308	1 - MA - VO - 15-44	25.0	2.984	36.724	1.468	6/27/84
82-309	1 - MA - VO - 45+	15.5	3.003	21.251	1.371	6/27/84
82-310	1 - EN - VO - 0-14	12.7	3.007	10.162	.800	6/28/84
82-311	1 - EN - VO - 15-44	20.8	2.931	9.109	.437	6/28/84
82-312	1 - EN - VO - 45+	18.6	2.852	5.983	.321	6/28/84
82-313	1 - WN - VO - 0-14	18.9	3.007	34.420	1.821	6/29/84
82-314	1 - WN - VO - 15-44	21.6	2.946	3.859	.178	6/29/84
82-315	1 - WN - VO - 45+	21.6	2.953	4.281	.198	7/2/84
82-316	1 - SA - VO - 0-14	12.6	3.055	8.043	.638	7/3/84
82-317	1 - SA - VO - 15-44	22.2	3.186	12.525	.564	7/3/84
82-318	1 - SA - VO - 45+	15.4	3.138	22.899	1.486	7/3/84
82-319	1 - ES - VO - 0-14	25.6	3.003	5.419	.211	7/9/84
82-320	1 - ES - VO - 15-44	19.0	3.152	14.718	.774	7/9/84
82-321	1 - ES - VO - 45+	20.6	3.092	9.877	.479	7/9/84
82-322	1 - WS - VO - 0-14	6.0	3.068	4.449	.741	7/11/84
82-323	1 - WS - VO - 15-44	22.4	2.942	10.351	.462	7/11/84
82-324	1 - WS - VO - 45+	22.0	2.961	13.796	.627	7/11/84
82-325	1 - MO - VO - 0-14	5.1	3.129	2.123	.416	7/11/84
82-326	1 - MO - VO - 15-44	18.8	3.055	4.348	.231	7/12/84
82-327	1 - MO - VO - 45+	22.4	3.227	7.511	.335	7/12/84
82-328	2 - MA - VO - 0-14	18.1	3.072	3.621	.200	7/12/84
82-329	2 - MA - VO - 15-44	25.3	3.105	6.170	.243	7/13/84
82-330	2 - MA - VO - 45+	17.8	3.269	10.112	.568	7/13/84
82-331	2 - EN - VO - 0-14	17.3	2.976	2.026	.117	7/13/84
82-332	2 - EN - VO - 15-44	21.1	2.816	27.491	1.302	7/16/84
82-333	2 - EN - VO - 45+	22.6	ND	ND	ND	7/16/84
82-334	2 - WN - VO - 45+	18.3	2.885	7.126	.389	7/16/84
82-335	2 - SA - VO - 0-14	16.7	2.771	41.443	2.481	7/17/84
82-336	2 - SA - VO - 15-44	18.7	2.844	70.908	3.791	7/17/84
82-337	2 - SA - VO - 45+	23.2	2.861	9.395	.404	7/17/84
82-338	2 - ES - VO - 15-44	24.3	2.809	7.265	.298	7/18/84
82-339	2 - ES - VO - 45+	19.3	2.850	20.211	1.047	7/20/84
82-340	2 - WS - VO - 15-44	21.9	2.796	16.058	.733	7/18/84
82-341	3 - EN - VO - 15-44	19.6	2.792	5.198	.265	7/18/84
82-342	3 - EN - VO - 45+	21.4	2.810	12.947	.605	7/18/84
82-343	3 - SA - VO - 15-44	10.1	2.861	14.836	1.468	7/20/84
82-344	3 - SA - VO - 45+	13.8	2.918	15.842	1.148	7/20/84
82-345	4 - SA - VO - 15-44	17.8	2.861	13.753	.772	7/20/84
82-346	4 - SA - VO - 45+	11.6	2.947	3.285	.283	7/20/84

Appendix A-9

FY82 VOA Adipose Composite Summary

CAS No.: 124-11-

Data Report - Nonenes (1-Nonene) Fraction: VC

RRf: 0.21

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	1.945	275.371	18.358	6/19/84
82-302	1 - PA - VO - 15-44	17.4	1.901	240.382	13.815	6/20/84
82-303	1 - PA - VO - 45+	20.7	1.894	335.653	16.215	6/20/84
82-304	1 - NE - VO - 0-14	20.0	1.910	160.121	8.006	6/20/84
82-305	1 - NE - VO - 15-44	23.6	1.863	381.242	16.154	6/21/84
82-306	1 - NE - VO - 45+	25.5	1.878	219.628	8.612	6/26/84
82-307	1 - MA - VO - 0-14	20.3	1.909	205.781	10.137	6/27/84
82-308	1 - MA - VO - 15-44	25.0	1.895	177.356	7.094	6/27/84
82-309	1 - MA - VO - 45+	15.5	1.910	213.251	13.758	6/27/84
82-310	1 - EN - VO - 0-14	12.7	1.917	62.186	4.896	6/28/84
82-311	1 - EN - VO - 15-44	20.8	1.904	109.071	5.243	6/28/84
82-312	1 - EN - VO - 45+	18.6	1.860	94.078	5.058	6/28/84
82-313	1 - WN - VO - 0-14	18.9	1.910	163.745	8.663	6/29/84
82-314	1 - WN - VO - 15-44	21.6	1.877	137.709	6.375	6/29/84
82-315	1 - WN - VO - 45+	21.6	1.857	91.438	4.233	7/2/84
82-316	1 - SA - VO - 0-14	12.6	1.944	555.272	44.069	7/3/84
82-317	1 - SA - VO - 15-44	22.2	2.020	291.532	13.132	7/3/84
82-318	1 - SA - VO - 45+	15.4	2.004	360.057	23.380	7/3/84
82-319	1 - ES - VO - 0-14	25.6	1.960	977.277	38.174	7/9/84
82-320	1 - ES - VO - 15-44	19.0	2.016	495.604	26.084	7/9/84
82-321	1 - ES - VO - 45+	20.6	1.979	410.324	19.918	7/9/84
82-322	1 - WS - VO - 0-14	6.0	1.984	544.895	90.815	7/11/84
82-323	1 - WS - VO - 15-44	22.4	1.900	215.792	9.633	7/11/84
82-324	1 - WS - VO - 45+	22.0	1.907	229.972	10.453	7/11/84
82-325	1 - MO - VO - 0-14	5.1	1.995	23.191	4.547	7/11/84
82-326	1 - MO - VO - 15-44	18.8	1.968	417.887	22.228	7/12/84
82-327	1 - MO - VO - 45+	22.4	2.084	138.810	6.196	7/12/84
82-328	2 - MA - VO - 0-14	18.1	1.943	145.961	8.064	7/12/84
82-329	2 - MA - VO - 15-44	25.3	2.008	281.974	11.145	7/13/84
82-330	2 - MA - VO - 45+	17.8	2.081	209.512	11.770	7/13/84
82-331	2 - EN - VO - 0-14	17.3	1.926	282.243	16.314	7/13/84
82-332	2 - EN - VO - 15-44	21.1	1.852	171.198	8.113	7/16/84
82-333	2 - EN - VO - 45+	22.6	1.824	162.628	7.195	7/16/84
82-334	2 - WN - VO - 45+	18.3	1.867	166.119	9.077	7/16/84
82-335	2 - SA - VO - 0-14	16.7	1.820	241.669	14.471	7/17/84
82-336	2 - SA - VO - 15-44	18.7	1.851	543.256	29.051	7/17/84
82-337	2 - SA - VO - 45+	23.2	1.865	332.522	14.332	7/17/84
82-338	2 - ES - VO - 15-44	24.3	1.838	190.270	7.830	7/18/84
82-339	2 - ES - VO - 45+	19.3	1.847	223.354	11.572	7/20/84
82-340	2 - WS - VO - 15-44	21.9	1.828	104.246	4.760	7/18/84
82-341	3 - EN - VO - 15-44	19.6	1.821	145.024	7.399	7/18/84
82-342	3 - EN - VO - 45+	21.4	1.831	270.228	12.627	7/18/84
82-343	3 - SA - VO - 15-44	10.1	1.854	231.211	22.892	7/20/84
82-344	3 - SA - VO - 45+	13.8	1.899	812.598	58.883	7/20/84
82-345	4 - SA - VO - 15-44	17.8	1.854	617.080	34.667	7/20/84
82-346	4 - SA - VO - 45+	11.6	1.924	169.950	14.650	7/20/84

Appendix A-10

FY82 VOA Adipose Composite Summary

CAS No.: 1669-44-9

Data Report - 3-Octen-2-one

Fraction: VOA

RRf: 0.010

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	3.160	296.474	19.764	6/19/84
82-302	1 - PA - VO - 15-44	17.4	3.030	104.800	6.023	6/20/84
82-303	1 - PA - VO - 45+	20.7	3.018	29.316	1.416	6/20/84
82-304	1 - NE - VO - 0-14	20.0	3.000	265.657	13.282	6/20/84
82-305	1 - NE - VO - 15-44	23.6	2.977	479.644	20.323	6/21/84
82-306	1 - NE - VO - 45+	25.5	2.963	424.655	16.653	6/26/84
82-307	1 - MA - VO - 0-14	20.3	3.113	33.322	1.641	6/27/84
82-308	1 - MA - VO - 15-44	25.0	3.081	116.204	4.648	6/27/84
82-309	1 - MA - VO - 45+	15.5	3.108	170.634	11.008	6/27/84
82-310	1 - EN - VO - 0-14	12.7	3.824	141.092	11.109	6/28/84
82-311	1 - EN - VO - 15-44	20.8	3.722	104.098	5.004	6/28/84
82-312	1 - EN - VO - 45+	18.6	2.948	117.966	6.342	6/28/84
82-313	1 - WN - VO - 0-14	18.9	3.824	132.310	7.000	6/29/84
82-314	1 - WN - VO - 15-44	21.6	3.057	27.014	1.250	6/29/84
82-315	1 - WN - VO - 45+	21.6	ND	ND	ND	7/2/84
82-316	1 - SA - VO - 0-14	12.6	3.170	1022.786	81.173	7/3/84
82-317	1 - SA - VO - 15-44	22.2	3.315	182.773	8.233	7/3/84
82-318	1 - SA - VO - 45+	15.4	3.257	138.485	8.992	7/3/84
82-319	1 - ES - VO - 0-14	25.6	3.121	184.541	7.208	7/9/84
82-320	1 - ES - VO - 15-44	19.0	3.279	126.598	6.663	7/9/84
82-321	1 - ES - VO - 45+	20.6	3.208	121.924	5.918	7/9/84
82-322	1 - WS - VO - 0-14	6.0	3.188	865.808	144.301	7/11/84
82-323	1 - WS - VO - 15-44	22.4	3.049	548.157	24.471	7/11/84
82-324	1 - WS - VO - 45+	22.0	3.065	196.100	8.913	7/11/84
82-325	1 - MO - VO - 0-14	5.1	3.263	155.395	30.469	7/11/84
82-326	1 - MO - VO - 15-44	18.8	3.191	270.497	14.388	7/12/84
82-327	1 - MO - VO - 45+	22.4	3.367	504.488	22.521	7/12/84
82-328	2 - MA - VO - 0-14	18.1	3.180	73.088	4.038	7/12/84
82-329	2 - MA - VO - 15-44	25.3	3.238	154.011	6.087	7/13/84
82-330	2 - MA - VO - 45+	17.8	3.423	166.130	9.333	7/13/84
82-331	2 - EN - VO - 0-14	17.3	3.089	208.795	12.069	7/13/84
82-332	2 - EN - VO - 15-44	21.1	2.917	67.476	3.197	7/16/84
82-333	2 - EN - VO - 45+	22.6	ND	ND	ND	7/16/84
82-334	2 - WN - VO - 45+	18.3	2.988	31.665	1.730	7/16/84
82-335	2 - SA - VO - 0-14	16.7	2.876	758.123	45.396	7/17/84
82-336	2 - SA - VO - 15-44	18.7	2.942	399.827	21.381	7/17/84
82-337	2 - SA - VO - 45+	23.2	2.960	65.396	2.818	7/17/84
82-338	2 - ES - VO - 15-44	24.3	2.910	77.709	3.197	7/18/84
82-339	2 - ES - VO - 45+	19.3	2.952	85.373	4.423	7/20/84
82-340	2 - WS - VO - 15-44	21.9	2.892	50.793	2.319	7/18/84
82-341	3 - EN - VO - 15-44	19.6	2.889	70.602	3.602	7/18/84
82-342	3 - EN - VO - 45+	21.4	2.906	141.031	6.590	7/18/84
82-343	3 - SA - VO - 15-44	10.1	2.967	252.322	24.982	7/20/84
82-344	3 - SA - VO - 45+	13.8	3.018	219.589	15.912	7/20/84
82-345	4 - SA - VO - 15-44	17.8	2.959	399.743	22.457	7/20/84
82-346	4 - SA - VO - 45+	11.6	3.056	133.775	11.532	7/20/84

Appendix A-11

FY82 VOA Adipose Composite Summary

CAS No.: 123-51-3

Data Report - Pentyl Alcohol (3-methyl-1-butanol)

Fraction: VOA

RRf: 0.020

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	1.117	128.485	8.565	6/19/84
82-302	1 - PA - VO - 15-44	17.4	1.125	81.837	4.703	6/20/84
82-303	1 - PA - VO - 45+	20.7	1.067	40.998	1.980	6/20/84
82-304	1 - NE - VO - 0-14	20.0	ND	ND	ND	6/20/84
82-305	1 - NE - VO - 15-44	23.6	1.110	349.769	14.820	6/21/84
82-306	1 - NE - VO - 45+	25.5	ND	ND	ND	6/26/84
82-307	1 - MA - VO - 0-14	20.3	1.094	35.650	1.756	6/27/84
82-308	1 - MA - VO - 15-44	25.0	1.111	37.860	1.514	6/27/84
82-309	1 - MA - VO - 45+	15.5	1.120	44.780	2.889	6/27/84
82-310	1 - EN - VO - 0-14	12.7	1.093	41.198	3.243	6/28/84
82-311	1 - EN - VO - 15-44	20.8	1.117	35.474	1.705	6/28/84
82-312	1 - EN - VO - 45+	18.6	ND	ND	ND	6/28/84
82-313	1 - WN - VO - 0-14	18.9	1.121	31.864	1.685	6/29/84
82-314	1 - WN - VO - 15-44	21.6	1.095	63.990	2.962	6/29/84
82-315	1 - WN - VO - 45+	21.6	1.146	7.648	.354	7/2/84
82-316	1 - SA - VO - 0-14	12.6	ND	ND	ND	7/3/84
82-317	1 - SA - VO - 15-44	22.2	1.190	92.669	4.174	7/3/84
82-318	1 - SA - VO - 45+	15.4	1.195	73.039	4.742	7/3/84
82-319	1 - ES - VO - 0-14	25.6	1.145	237.386	9.272	7/9/84
82-320	1 - ES - VO - 15-44	19.0	1.205	150.415	7.916	7/9/84
82-321	1 - ES - VO - 45+	20.6	1.100	63.423	3.078	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	ND	ND	ND	7/11/84
82-324	1 - WS - VO - 45+	22.0	1.126	236.147	10.733	7/11/84
82-325	1 - MO - VO - 0-14	5.1	ND	ND	ND	7/11/84
82-326	1 - MO - VO - 15-44	18.8	ND	ND	ND	7/12/84
82-327	1 - MO - VO - 45+	22.4	1.177	320.029	14.287	7/12/84
82-328	2 - MA - VO - 0-14	18.1	1.088	145.772	8.053	7/12/84
82-329	2 - MA - VO - 15-44	25.3	1.190	237.444	9.385	7/13/84
82-330	2 - MA - VO - 45+	17.8	1.179	199.842	11.227	7/13/84
82-331	2 - EN - VO - 0-14	17.3	1.139	95.985	5.548	7/13/84
82-332	2 - EN - VO - 15-44	21.1	1.140	59.177	2.804	7/16/84
82-333	2 - EN - VO - 45+	22.6	1.114	131.009	5.796	7/16/84
82-334	2 - WN - VO - 45+	18.3	1.121	67.062	3.664	7/16/84
82-335	2 - SA - VO - 0-14	16.7	ND	ND	ND	7/17/84
82-336	2 - SA - VO - 15-44	18.7	1.122	222.237	11.884	7/17/84
82-337	2 - SA - VO - 45+	23.2	1.116	142.719	6.151	7/17/84
82-338	2 - ES - VO - 15-44	24.3	1.118	68.954	2.837	7/18/84
82-339	2 - ES - VO - 45+	19.3	1.127	37.503	1.943	7/20/84
82-340	2 - WS - VO - 15-44	21.9	1.121	44.403	2.027	7/18/84
82-341	3 - EN - VO - 15-44	19.6	1.100	92.235	4.705	7/18/84
82-342	3 - EN - VO - 45+	21.4	1.100	89.607	4.187	7/18/84
82-343	3 - SA - VO - 15-44	10.1	1.109	86.051	8.519	7/20/84
82-344	3 - SA - VO - 45+	13.8	1.100	140.745	10.198	7/20/84
82-345	4 - SA - VO - 15-44	17.8	1.127	180.280	10.128	7/20/84
82-346	4 - SA - VO - 45+	11.6	1.128	93.730	8.080	7/20/84

Appendix A-12

FY82 VOA Adipose Composite Summary

CAS No.: 4292-92-6

Data Report - Pentyl cyclohexane

Fraction: VOA

RRf: 0.160

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	ND	ND	ND	6/19/84
82-302	1 - PA - VO - 15-44	17.4	ND	ND	ND	6/20/84
82-303	1 - PA - VO - 45+	20.7	ND	ND	ND	6/20/84
82-304	1 - NE - VO - 0-14	20.0	ND	ND	ND	6/20/84
82-305	1 - NE - VO - 15-44	23.6	ND	ND	ND	6/21/84
82-306	1 - NE - VO - 45+	25.5	3.485	7.216	.282	6/26/84
82-307	1 - MA - VO - 0-14	20.3	ND	ND	ND	6/27/84
82-308	1 - MA - VO - 15-44	25.0	ND	ND	ND	6/27/84
82-309	1 - MA - VO - 45+	15.5	ND	ND	ND	6/27/84
82-310	1 - EN - VO - 0-14	12.7	3.679	1.383	.108	6/28/84
82-311	1 - EN - VO - 15-44	20.8	ND	ND	ND	6/28/84
82-312	1 - EN - VO - 45+	18.6	ND	ND	ND	6/28/84
82-313	1 - WN - VO - 0-14	18.9	ND	ND	ND	6/29/84
82-314	1 - WN - VO - 15-44	21.6	ND	ND	ND	6/29/84
82-315	1 - WN - VO - 45+	21.6	ND	ND	ND	7/2/84
82-316	1 - SA - VO - 0-14	12.6	ND	ND	ND	7/3/84
82-317	1 - SA - VO - 15-44	22.2	3.908	1.257	.056	7/3/84
82-318	1 - SA - VO - 45+	15.4	ND	ND	ND	7/3/84
82-319	1 - ES - VO - 0-14	25.6	ND	ND	ND	7/9/84
82-320	1 - ES - VO - 15-44	19.0	ND	ND	ND	7/9/84
82-321	1 - ES - VO - 45+	20.6	ND	ND	ND	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	ND	ND	ND	7/11/84
82-324	1 - WS - VO - 45+	22.0	ND	ND	ND	7/11/84
82-325	1 - MO - VO - 0-14	5.1	ND	ND	ND	7/11/84
82-326	1 - MO - VO - 15-44	18.8	ND	ND	ND	7/12/84
82-327	1 - MO - VO - 45+	22.4	ND	ND	ND	7/12/84
82-328	2 - MA - VO - 0-14	18.1	ND	ND	ND	7/12/84
82-329	2 - MA - VO - 15-44	25.3	ND	ND	ND	7/13/84
82-330	2 - MA - VO - 45+	17.8	ND	ND	ND	7/13/84
82-331	2 - EN - VO - 0-14	17.3	ND	ND	ND	7/13/84
82-332	2 - EN - VO - 15-44	21.1	ND	ND	ND	7/16/84
82-333	2 - EN - VO - 45+	22.6	ND	ND	ND	7/16/84
82-334	2 - WN - VO - 45+	18.3	ND	ND	ND	7/16/84
82-335	2 - SA - VO - 0-14	16.7	ND	ND	ND	7/17/84
82-336	2 - SA - VO - 15-44	18.7	ND	ND	ND	7/17/84
82-337	2 - SA - VO - 45+	23.2	3.480	2.144	.092	7/17/84
82-338	2 - ES - VO - 15-44	24.3	3.428	.588	.024	7/18/84
82-339	2 - ES - VO - 45+	19.3	ND	ND	ND	7/20/84
82-340	2 - WS - VO - 15-44	21.9	3.403	1.615	.073	7/18/84
82-341	3 - EN - VO - 15-44	19.6	ND	ND	ND	7/18/84
82-342	3 - EN - VO - 45+	21.4	3.422	.423	.019	7/18/84
82-343	3 - SA - VO - 15-44	10.1	3.485	2.040	.202	7/20/84
82-344	3 - SA - VO - 45+	13.8	3.546	2.434	.176	7/20/84
82-345	4 - SA - VO - 15-44	17.8	3.481	2.521	.141	7/20/84
82-346	4 - SA - VO - 45+	11.6	ND	ND	ND	7/20/84

Appendix A-13

FY82 VOA Adipose Composite Summary

CAS No.: 79-01-6

Data Report - Trichloroethylene {Trichloroethene} Fraction: VOA

RRf: 0.335

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-301	1 - PA - VO - 0-14	15.0	ND	ND	ND	6/19/84
82-302	1 - PA - VO - 15-44	17.4	.602	.031	.001	6/20/84
82-303	1 - PA - VO - 45+	20.7	.605	.135	.006	6/20/84
82-304	1 - NE - VO - 0-14	20.0	.602	.113	.005	6/20/84
82-305	1 - NE - VO - 15-44	23.6	ND	ND	ND	6/21/84
82-306	1 - NE - VO - 45+	25.5	ND	ND	ND	6/26/84
82-307	1 - MA - VO - 0-14	20.3	ND	ND	ND	6/27/84
82-308	1 - MA - VO - 15-44	25.0	.602	.171	.006	6/27/84
82-309	1 - MA - VO - 45+	15.5	.603	.032	.002	6/27/84
82-310	1 - EN - VO - 0-14	12.7	.605	.046	.003	6/28/84
82-311	1 - EN - VO - 15-44	20.8	ND	ND	ND	6/28/84
82-312	1 - EN - VO - 45+	18.6	.599	.191	.010	6/28/84
82-313	1 - WN - VO - 0-14	18.9	ND	ND	ND	6/29/84
82-314	1 - WN - VO - 15-44	21.6	ND	ND	ND	6/29/84
82-315	1 - WN - VO - 45+	21.6	.610	.020	<.001	7/2/84
82-316	1 - SA - VO - 0-14	12.6	ND	ND	ND	7/3/84
82-317	1 - SA - VO - 15-44	22.2	ND	ND	ND	7/3/84
82-318	1 - SA - VO - 45+	15.4	.612	.070	.004	7/3/84
82-319	1 - ES - VO - 0-14	25.6	ND	ND	ND	7/9/84
82-320	1 - ES - VO - 15-44	19.0	ND	ND	ND	7/9/84
82-321	1 - ES - VO - 45+	20.6	ND	ND	ND	7/9/84
82-322	1 - WS - VO - 0-14	6.0	ND	ND	ND	7/11/84
82-323	1 - WS - VO - 15-44	22.4	ND	ND	ND	7/11/84
82-324	1 - WS - VO - 45+	22.0	ND	ND	ND	7/11/84
82-325	1 - MO - VO - 0-14	5.1	ND	ND	ND	7/11/84
82-326	1 - MO - VO - 15-44	18.8	ND	ND	ND	7/12/84
82-327	1 - MO - VO - 45+	22.4	ND	ND	ND	7/12/84
82-328	2 - MA - VO - 0-14	18.1	ND	ND	ND	7/12/84
82-329	2 - MA - VO - 15-44	25.3	.623	.095	.003	7/13/84
82-330	2 - MA - VO - 45+	17.8	ND	ND	ND	7/13/84
82-331	2 - EN - VO - 0-14	17.3	.593	.098	.005	7/13/84
82-332	2 - EN - VO - 15-44	21.1	.607	.176	.008	7/16/84
82-333	2 - EN - VO - 45+	22.6	.602	.161	.007	7/16/84
82-334	2 - WN - VO - 45+	18.3	.612	.099	.005	7/16/84
82-335	2 - SA - VO - 0-14	16.7	ND	ND	ND	7/17/84
82-336	2 - SA - VO - 15-44	18.7	ND	ND	ND	7/17/84
82-337	2 - SA - VO - 45+	23.2	ND	ND	ND	7/17/84
82-338	2 - ES - VO - 15-44	24.3	.607	.088	.003	7/18/84
82-339	2 - ES - VO - 45+	19.3	.607	.115	.006	7/20/84
82-340	2 - WS - VO - 15-44	21.9	.603	.082	.003	7/18/84
82-341	3 - EN - VO - 15-44	19.6	.607	.054	.002	7/18/84
82-342	3 - EN - VO - 45+	21.4	.609	.099	.004	7/18/84
82-343	3 - SA - VO - 15-44	10.1	.605	.044	.004	7/20/84
82-344	3 - SA - VO - 45+	13.8	ND	ND	ND	7/20/84
82-345	4 - SA - VO - 15-44	17.8	ND	ND	ND	7/20/84
82-346	4 - SA - VO - 45+	11.6	ND	ND	ND	7/20/84

APPENDIX B

6% FLORISIL FRACTION SEMIVOLATILE COMPOSITE SUMMARY REPORTS

Appendix B-1

FY82 6% SMV Adipose Composite Summary

CAS No.: 120-12-7

Data Report - Anthracene

Fraction: 6% SMV

RRf: 1.439

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/19/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/19/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/19/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/7/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/8/84
82-67	1 - SA - SV - 0-14	20.7	ND	ND	ND	5/11/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	6/1/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/5/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/6/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/6/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/5/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/5/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/4/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/12/84
82-83	1 - WS - SV - 15-44	22.7	1.002	.005	<.001	5/4/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/18/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/18/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/20/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/10/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/4/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/5/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/5/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/6/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/19/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/20/84
82-69	1 - SA - SV - 45+	20.0	ND	ND	ND	4/20/84
82-65	1 - WN - SV - 45+	22.5	ND	ND	ND	5/7/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/10/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	6/1/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/4/84
82-60	2 - EN - SV - 45+	26.2	ND	ND	ND	6/4/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/5/84
82-62	3 - EN - SV - 45+	23.2	ND	ND	ND	6/6/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/6/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/12/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/12/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/12/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/15/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/19/84
82-57	1 - EN - SV - 45+	19.8	ND	ND	ND	4/20/84

Appendix B-2

FY82 6% SMV Adipose Composite Summary

CAS No.: 92-52-4

Data Report - Biphenyl

Fraction: 6% SMV

RRf: 1.286

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/19/84
82-55	1 - BN - SV - 0-14	18.1	ND	ND	ND	4/19/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/19/84
82-63	1 - WN - SV - 0-14	23.4	.665	.009	<.001	5/7/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/8/84
82-67	1 - SA - SV - 0-14	20.7	.665	.026	.001	5/11/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	6/1/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/5/84
82-58	2 - BN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/6/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/6/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/5/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/5/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/4/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/12/84
82-83	1 - WS - SV - 15-44	22.7	.662	.014	<.001	5/4/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/18/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/18/84
82-56	1 - BN - SV - 15-44	21.6	ND	ND	ND	4/20/84
82-78	1 - ES - SV - 15-44	19.9	.674	.012	<.001	5/10/84
82-59	2 - BN - SV - 15-44	21.4	ND	ND	ND	6/4/84
82-61	3 - BN - SV - 15-44	20.2	ND	ND	ND	6/5/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/5/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/6/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/19/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/20/84
82-69	1 - SA - SV - 45+	20.0	.667	.017	<.001	4/20/84
82-65	1 - WN - SV - 45+	22.5	.667	.014	<.001	5/7/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	.662	.014	<.001	5/10/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	6/1/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/4/84
82-60	2 - BN - SV - 45+	26.2	ND	ND	ND	6/4/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/5/84
82-62	3 - BN - SV - 45+	23.2	ND	ND	ND	6/6/84
82-81	2 - ES - SV - 45+	21.1	.656	.022	.001	6/6/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/12/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/12/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/12/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/15/84
82-48	1 - PA - SV - 45+	22.0	.672	.009	<.001	4/19/84
82-57	1 - BN - SV - 45+	19.8	ND	ND	ND	4/20/84

Appendix B-3

FY82 6% SMV Adipose Composite Summary

CAS No.: 99-87-6

Data Report - Cymene (isopropyltoluene)

Fraction: 6% SMV

RRf: 1.620

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	.342	.005	<.001	4/19/84
82-55	1 - EN - SV - 0-14	18.1	.344	.008	<.001	4/19/84
82-46	1 - PA - SV - 0-14	19.7	.344	.011	<.001	4/19/84
82-63	1 - WN - SV - 0-14	23.4	.331	.016	<.001	5/7/84
82-82	1 - WS - SV - 0-14	11.1	.327	.010	<.001	5/8/84
82-67	1 - SA - SV - 0-14	20.7	.330	.080	.003	5/11/84
82-77	1 - ES - SV - 0-14	28.1	.292	.034	.001	6/1/84
82-70	2 - SA - SV - 0-14	19.1	.293	.034	.001	6/5/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	.325	.002	<.001	6/13/84
82-42	1 - NE - SV - 0-14	19.1	.292	.001	<.001	4/6/84
82-49	1 - MA - SV - 0-14	23.0	.332	.002	<.001	4/6/84
82-43	1 - NE - SV - 15-44	21.9	.328	.014	<.001	4/5/84
82-50	1 - MA - SV - 15-44	25.2	.331	.011	<.001	4/5/84
82-64	1 - WN - SV - 15-44	20.6	.345	.018	<.001	5/4/84
82-53	2 - MA - SV - 15-44	26.1	.329	.007	<.001	6/12/84
82-83	1 - WS - SV - 15-44	22.7	.325	.029	.001	5/4/84
82-85	2 - WS - SV - 15-44	21.9	.317	.006	<.001	6/18/84
82-71	2 - SA - SV - 15-44	19.5	.322	.046	.002	6/18/84
82-56	1 - EN - SV - 15-44	21.6	.342	.018	<.001	4/20/84
82-78	1 - ES - SV - 15-44	19.9	.347	.026	.001	5/10/84
82-59	2 - EN - SV - 15-44	21.4	.295	.007	<.001	6/4/84
82-61	3 - EN - SV - 15-44	20.2	.295	.018	<.001	6/5/84
82-73	3 - SA - SV - 15-44	17.9	.277	.101	.005	6/5/84
82-75	4 - SA - SV - 15-44	18.2	.281	.051	.002	6/6/84
82-37	1 - MO - SV - 15-44	18.3	.338	.009	<.001	4/19/84
82-68	1 - SA - SV - 15-44	26.4	.344	.087	.003	4/20/84
82-69	1 - SA - SV - 45+	20.0	.342	.067	.003	4/20/84
82-65	1 - WN - SV - 45+	22.5	.331	.017	<.001	5/7/84
82-84	1 - WS - SV - 45+	22.4	.345	.027	.001	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	.331	.018	<.001	5/10/84
82-51	1 - MA - SV - 45+	16.2	.316	.009	<.001	6/1/84
82-72	2 - SA - SV - 45+	26.1	.338	.053	.002	6/4/84
82-60	2 - EN - SV - 45+	26.2	.282	.041	.001	6/4/84
82-66	2 - WN - SV - 45+	21.4	.293	.009	<.001	6/5/84
82-62	3 - EN - SV - 45+	23.2	.286	.027	.001	6/6/84
82-81	2 - ES - SV - 45+	21.1	.288	.058	.002	6/6/84
82-74	3 - SA - SV - 45+	18.0	.311	.031	.001	6/12/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/12/84
82-54	2 - MA - SV - 45+	18.1	.317	.027	.001	6/12/84
82-44	1 - NE - SV - 45+	26.7	.327	.009	<.001	4/15/84
82-48	1 - PA - SV - 45+	22.0	.348	.011	<.001	4/19/84
82-57	1 - EN - SV - 45+	19.8	.344	.017	<.001	4/20/84

Appendix B-4

FY82 6% SMV Adipose Composite Summary

CAS No.: 132-64-9

Data Report - Dibenzofuran

Fraction: 6% SMV

RRf: 1.272

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/19/84
82-55	1 - BN - SV - 0-14	18.1	ND	ND	ND	4/19/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/19/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/7/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/8/84
82-67	1 - SA - SV - 0-14	20.7	.786	.011	<.001	5/11/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	6/1/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/5/84
82-58	2 - BN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/6/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/6/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/5/84
82-50	1 - MA - SV - 15-44	25.2	.793	.014	<.001	4/5/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/4/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/12/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/4/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/18/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/18/84
82-56	1 - BN - SV - 15-44	21.6	ND	ND	ND	4/20/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/10/84
82-59	2 - BN - SV - 15-44	21.4	ND	ND	ND	6/4/84
82-61	3 - BN - SV - 15-44	20.2	ND	ND	ND	6/5/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/5/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/6/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/19/84
82-68	1 - SA - SV - 15-44	26.4	.788	.023	<.001	4/20/84
82-69	1 - SA - SV - 45+	20.0	ND	ND	ND	4/20/84
82-65	1 - WN - SV - 45+	22.5	ND	ND	ND	5/7/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/10/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	6/1/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/4/84
82-60	2 - BN - SV - 45+	26.2	ND	ND	ND	6/4/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/5/84
82-62	3 - BN - SV - 45+	23.2	ND	ND	ND	6/6/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/6/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/12/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/12/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/12/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/15/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/19/84
82-57	1 - BN - SV - 45+	19.8	ND	ND	ND	4/20/84

Appendix B-5

FY82 6% SMV Adipose Composite Summary

CAS No.: 101-84-8

Data Report - Diphenyl ether (1,1'-Oxybisbenzene) Fraction: 6% SMV

RRf: 0.658

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/19/84
82-55	1 - BN - SV - 0-14	18.1	.689	.021	.001	4/19/84
82-46	1 - PA - SV - 0-14	19.7	.688	.053	.002	4/19/84
82-63	1 - WN - SV - 0-14	23.4	.684	.064	.002	5/7/84
82-82	1 - WS - SV - 0-14	11.1	.683	.059	.005	5/8/84
82-67	1 - SA - SV - 0-14	20.7	.684	.941	.045	5/11/84
82-77	1 - ES - SV - 0-14	28.1	.678	.480	.017	6/1/84
82-70	2 - SA - SV - 0-14	19.1	.678	.111	.005	6/5/84
82-58	2 - BN - SV - 0-14	21.2	.682	.030	.001	6/5/84
82-52	2 - MA - SV - 0-14	20.2	.683	.048	.002	6/13/84
82-42	1 - NE - SV - 0-14	19.1	.679	.004	<.001	4/6/84
82-49	1 - MA - SV - 0-14	23.0	.696	.085	.003	4/6/84
82-43	1 - NE - SV - 15-44	21.9	.693	.079	.003	4/5/84
82-50	1 - MA - SV - 15-44	25.2	.695	.252	.010	4/5/84
82-64	1 - WN - SV - 15-44	20.6	.693	.540	.026	5/4/84
82-53	2 - MA - SV - 15-44	26.1	.684	.334	.012	6/12/84
82-83	1 - WS - SV - 15-44	22.7	.681	.236	.010	5/4/84
82-85	2 - WS - SV - 15-44	21.9	.674	.188	.008	6/18/84
82-71	2 - SA - SV - 15-44	19.5	.680	.373	.019	6/18/84
82-56	1 - BN - SV - 15-44	21.6	.689	.208	.009	4/20/84
82-78	1 - ES - SV - 15-44	19.9	.693	.326	.016	5/10/84
82-59	2 - BN - SV - 15-44	21.4	.678	.034	.001	6/4/84
82-61	3 - BN - SV - 15-44	20.2	.680	.073	.003	6/5/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/5/84
82-75	4 - SA - SV - 15-44	18.2	.677	.208	.011	6/6/84
82-37	1 - MO - SV - 15-44	18.3	.687	.239	.013	4/19/84
82-68	1 - SA - SV - 15-44	26.4	.688	1.214	.045	4/20/84
82-69	1 - SA - SV - 45+	20.0	.686	.594	.029	4/20/84
82-65	1 - WN - SV - 45+	22.5	.686	.538	.023	5/7/84
82-84	1 - WS - SV - 45+	22.4	.692	.718	.032	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	.781	.139	.006	5/10/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	6/1/84
82-72	2 - SA - SV - 45+	26.1	.671	.607	.023	6/4/84
82-60	2 - BN - SV - 45+	26.2	.675	.260	.009	6/4/84
82-66	2 - WN - SV - 45+	21.4	.677	.124	.005	6/5/84
82-62	3 - BN - SV - 45+	23.2	.676	.286	.012	6/6/84
82-81	2 - ES - SV - 45+	21.1	.676	.171	.008	6/6/84
82-74	3 - SA - SV - 45+	18.0	.675	.075	.004	6/12/84
82-76	4 - SA - SV - 45+	17.6	.674	.049	.002	6/12/84
82-54	2 - MA - SV - 45+	18.1	.678	.117	.006	6/12/84
82-44	1 - NE - SV - 45+	26.7	.694	.097	.003	4/15/84
82-48	1 - PA - SV - 45+	22.0	.690	.134	.006	4/19/84
82-57	1 - BN - SV - 45+	19.8	.689	.212	.010	4/20/84

Appendix B-6

FY82 6% SMV Adipose Composite Summary

CAS No.: 138-86-3

Data Report - Limonene

Fraction: 6% SMV

RRf: 0.150

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	.346	.178	.019	4/19/84
82-55	1 - EN - SV - 0-14	18.1	.348	.084	.004	4/19/84
82-46	1 - PA - SV - 0-14	19.7	.347	.806	.040	4/19/84
82-63	1 - WN - SV - 0-14	23.4	.335	.353	.015	5/7/84
82-82	1 - WS - SV - 0-14	11.1	.331	.077	.006	5/8/84
82-67	1 - SA - SV - 0-14	20.7	.334	.250	.012	5/11/84
82-77	1 - ES - SV - 0-14	28.1	.296	.382	.013	6/1/84
82-70	2 - SA - SV - 0-14	19.1	.297	.331	.017	6/5/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	.327	.027	.001	6/13/84
82-42	1 - NE - SV - 0-14	19.1	.296	.007	<.001	4/6/84
82-49	1 - MA - SV - 0-14	23.0	.337	.023	.001	4/6/84
82-43	1 - NE - SV - 15-44	21.9	.333	.184	.008	4/5/84
82-50	1 - MA - SV - 15-44	25.2	.336	.410	.016	4/5/84
82-64	1 - WN - SV - 15-44	20.6	.349	.385	.018	5/4/84
82-53	2 - MA - SV - 15-44	26.1	.333	.126	.004	6/12/84
82-83	1 - WS - SV - 15-44	22.7	.329	.272	.012	5/4/84
82-85	2 - WS - SV - 15-44	21.9	.319	.146	.006	6/18/84
82-71	2 - SA - SV - 15-44	19.5	.326	.962	.049	6/18/84
82-56	1 - EN - SV - 15-44	21.6	.346	.235	.010	4/20/84
82-78	1 - ES - SV - 15-44	19.9	.351	.392	.019	5/10/84
82-59	2 - EN - SV - 15-44	21.4	.299	.106	.004	6/4/84
82-61	3 - EN - SV - 15-44	20.2	.298	.222	.010	6/5/84
82-73	3 - SA - SV - 15-44	17.9	.281	.555	.031	6/5/84
82-75	4 - SA - SV - 15-44	18.2	.285	.398	.021	6/6/84
82-37	1 - MO - SV - 15-44	18.3	.342	.067	.003	4/19/84
82-68	1 - SA - SV - 15-44	26.4	.348	.423	.016	4/20/84
82-69	1 - SA - SV - 45+	20.0	.345	.957	.047	4/20/84
82-65	1 - WN - SV - 45+	22.5	.335	.299	.013	5/7/84
82-84	1 - WS - SV - 45+	22.4	.349	.382	.017	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	.335	.146	.006	5/10/84
82-51	1 - MA - SV - 45+	16.2	.320	.313	.019	6/1/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/4/84
82-60	2 - EN - SV - 45+	26.2	.286	.477	.018	6/4/84
82-66	2 - WN - SV - 45+	21.4	.297	.154	.007	6/5/84
82-62	3 - EN - SV - 45+	23.2	.289	.266	.011	6/6/84
82-81	2 - ES - SV - 45+	21:1	.292	.984	.046	6/6/84
82-74	3 - SA - SV - 45+	18.0	.315	.306	.017	6/12/84
82-76	4 - SA - SV - 45+	17.6	.314	.271	.015	6/12/84
82-54	2 - MA - SV - 45+	18.1	.321	.716	.039	6/12/84
82-44	1 - NE - SV - 45+	26.7	.331	.149	.005	4/15/84
82-48	1 - PA - SV - 45+	22.0	.352	.347	.015	4/19/84
82-57	1 - EN - SV - 45+	19.8	.347	.276	.013	4/20/84

Appendix B-7

FY82 6% SMV Adipose Composite Summary

CAS No.: 94-59-7

Data Report - Safrole

Fraction: 6% SMV

RRf: 0.478

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/19/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/19/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/19/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/7/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/8/84
82-67	1 - SA - SV - 0-14	20.7	ND	ND	ND	5/11/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	6/1/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/5/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/6/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/6/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/5/84
82-50	1 - MA - SV - 15-44	25.2	.593	.011	<.001	4/5/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/4/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/12/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/4/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/18/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/18/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/20/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/10/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/4/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/5/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/5/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/6/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/19/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/20/84
82-69	1 - SA - SV - 45+	20.0	ND	ND	ND	4/20/84
82-65	1 - WN - SV - 45+	22.5	ND	ND	ND	5/7/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/10/84
82-51	1 - MA - SV - 45+	16.2	.572	.033	.002	6/1/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/4/84
82-60	2 - EN - SV - 45+	26.2	ND	ND	ND	6/4/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/5/84
82-62	3 - EN - SV - 45+	23.2	ND	ND	ND	6/6/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/6/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/12/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/12/84
82-54	2 - MA - SV - 45+	18.1	.572	1.150	.063	6/12/84
82-44	1 - NE - SV - 45+	26.7	.590	.102	.003	4/15/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/19/84
82-57	1 - EN - SV - 45+	19.8	ND	ND	ND	4/20/84

Appendix B-8

FY82 6% SMV Adipose Composite Summary

CAS No.: 95-63-6

Data Report - 1,2,4-Trimethylbenzene

Fraction: 6% SMV

RRf: 1.220

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	.315	.051	.005	4/19/84
82-55	1 - EN - SV - 0-14	18.1	.320	.037	.002	4/19/84
82-46	1 - PA - SV - 0-14	19.7	.316	.105	.005	4/19/84
82-63	1 - WN - SV - 0-14	23.4	.305	.026	.001	5/7/84
82-82	1 - WS - SV - 0-14	11.1	.300	.047	.004	5/8/84
82-67	1 - SA - SV - 0-14	20.7	.305	1.080	.052	5/11/84
82-77	1 - ES - SV - 0-14	28.1	.263	.084	.003	6/1/84
82-70	2 - SA - SV - 0-14	19.1	.262	.115	.006	6/5/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	.297	.028	.001	6/13/84
82-42	1 - NE - SV - 0-14	19.1	.261	.016	<.001	4/6/84
82-49	1 - MA - SV - 0-14	23.0	.301	.037	.001	4/6/84
82-43	1 - NE - SV - 15-44	21.9	.298	.045	.002	4/5/84
82-50	1 - MA - SV - 15-44	25.2	.303	.040	.001	4/5/84
82-64	1 - WN - SV - 15-44	20.6	.318	.039	.001	5/4/84
82-53	2 - MA - SV - 15-44	26.1	.302	.057	.002	6/12/84
82-83	1 - WS - SV - 15-44	22.7	.300	.058	.002	5/4/84
82-85	2 - WS - SV - 15-44	21.9	.289	.010	<.001	6/18/84
82-71	2 - SA - SV - 15-44	19.5	.296	.541	.027	6/18/84
82-56	1 - EN - SV - 15-44	21.6	.316	.068	.003	4/20/84
82-78	1 - ES - SV - 15-44	19.9	.321	.060	.003	5/10/84
82-59	2 - EN - SV - 15-44	21.4	.263	.010	<.001	6/4/84
82-61	3 - EN - SV - 15-44	20.2	.265	.037	.001	6/5/84
82-73	3 - SA - SV - 15-44	17.9	.247	.764	.042	6/5/84
82-75	4 - SA - SV - 15-44	18.2	.251	.409	.022	6/6/84
82-37	1 - MO - SV - 15-44	18.3	.312	.024	.001	4/19/84
82-68	1 - SA - SV - 15-44	26.4	.320	.787	.029	4/20/84
82-69	1 - SA - SV - 45+	20.0	.317	.618	.030	4/20/84
82-65	1 - WN - SV - 45+	22.5	.304	.093	.004	5/7/84
82-84	1 - WS - SV - 45+	22.4	.319	.070	.003	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	.304	.054	.002	5/10/84
82-51	1 - MA - SV - 45+	16.2	.289	.040	.002	6/1/84
82-72	2 - SA - SV - 45+	26.1	.273	.132	.005	6/4/84
82-60	2 - EN - SV - 45+	26.2	.250	.051	.001	6/4/84
82-66	2 - WN - SV - 45+	21.4	.263	.015	<.001	6/5/84
82-62	3 - EN - SV - 45+	23.2	.256	.073	.003	6/6/84
82-81	2 - ES - SV - 45+	21.1	.261	.023	.001	6/6/84
82-74	3 - SA - SV - 45+	18.0	.282	.306	.017	6/12/84
82-76	4 - SA - SV - 45+	17.6	.283	.031	.001	6/12/84
82-54	2 - MA - SV - 45+	18.1	.289	.062	.003	6/12/84
82-44	1 - NE - SV - 45+	26.7	.297	.052	.001	4/15/84
82-48	1 - PA - SV - 45+	22.0	.323	.030	.001	4/19/84
82-57	1 - EN - SV - 45+	19.8	.318	.062	.003	4/20/84

Appendix B-9

FY82 6% SMV Adipose Composite Summary

CAS No.: 87-62-7

Data Report - 2,6-Xylidine

Fraction: 6% SMV

RRf: 0.811

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/19/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/19/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/19/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/7/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/8/84
82-67	1 - SA - SV - 0-14	20.7	ND	ND	ND	5/11/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	6/1/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/5/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/5/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/6/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/6/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/5/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/5/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/4/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/12/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/4/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/18/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/18/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/20/84
82-78	1 - ES - SV - 15-44	19.9	.479	.014	<.001	5/10/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/4/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/5/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/5/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/6/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/19/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/20/84
82-69	1 - SA - SV - 45+	20.0	.471	.005	<.001	4/20/84
82-65	1 - WN - SV - 45+	22.5	.467	.291	.012	5/7/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/7/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/10/84
82-41	1 - MO - SV - 45+	21.0	.464	.422	.020	5/10/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	6/1/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/4/84
82-60	2 - EN - SV - 45+	26.2	.437	.198	.007	6/4/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/5/84
82-62	3 - EN - SV - 45+	23.2	.440	.328	.014	6/6/84
82-81	2 - ES - SV - 45+	21.1	.442	.036	.001	6/6/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/12/84
82-76	4 - SA - SV - 45+	17.6	.450	.318	.018	6/12/84
82-54	2 - MA - SV - 45+	18.1	.456	.008	<.001	6/12/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/15/84
82-48	1 - PA - SV - 45+	22.0	.479	.207	.009	4/19/84
82-57	1 - EN - SV - 45+	19.8	.475	.050	.002	4/20/84

APPENDIX C

15/50% FLORISIL FRACTION SEMIVOLATILE COMPOSITE SUMMARY REPORTS

Appendix C-1

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 103-23-1

Data Report - Bis(2-ethylhexyl)adipate

Fraction: 15/50% SMV

RRf: 0.733

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	1.363	.124	.006	4/26/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/14/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/24/84
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/24/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/25/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/10/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	5/14/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/14/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	ND	ND	ND	4/27/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/18/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/18/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/16/84
82-71	2 - SA - SV - 15-44	19.5	1.379	.551	.028	6/13/84
82-53	2 - MA - SV - 15-44	26.1	1.379	1.987	.076	6/13/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/9/84
82-85	2 - WS - SV - 15-44	21.9	1.379	2.840	.129	6/15/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/14/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/25/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/11/84
82-56	1 - EN - SV - 15-44	21.6	1.360	.053	.002	4/26/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/14/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/24/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/16/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/25/84
82-57	1 - EN - SV - 45+	19.8	ND	ND	ND	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/16/84
82-62	3 - EN - SV - 45+	23.2	ND	ND	ND	6/16/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/15/84
82-60	2 - EN - SV - 45+	26.2	ND	ND	ND	6/14/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/14/84
82-79	1 - ES - SV - 45+	20.7	1.373	3.426	.165	5/14/84
82-69	1 - SA - SV - 45+	20.0	1.364	.085	.004	4/24/84
82-65	1 - WN - SV - 45+	22.5	ND	ND	ND	5/10/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/13/84
82-72	2 - SA - SV - 45+	26.1	1.370	.864	.033	6/14/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/10/84

Appendix C-2

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 85-70-1

Data Report - Butyl glycol butyl phthalate

Fraction: 15/50% SMV

RRf: 1.330

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	ND	ND	ND	4/26/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/14/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/24/84
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/24/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/25/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/10/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	5/14/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/14/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	ND	ND	ND	4/27/84
82-61	3 - EN - SV - 15-44	20.2	1.333	.053	.002	6/18/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/18/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/16/84
82-71	2 - SA - SV - 15-44	19.5	1.335	1.281	.065	6/13/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/13/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/9/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/15/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/14/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/25/84
82-64	1 - WN - SV - 15-44	20.6	1.326	1.873	.090	5/11/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/26/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/14/84
82-68	1 - SA - SV - 15-44	26.4	1.326	.736	.027	4/24/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/16/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/25/84
82-57	1 - EN - SV - 45+	19.8	ND	ND	ND	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/16/84
82-62	3 - EN - SV - 45+	23.2	1.335	.267	.011	6/16/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/15/84
82-60	2 - EN - SV - 45+	26.2	1.329	.037	.001	6/14/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/14/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/14/84
82-69	1 - SA - SV - 45+	20.0	ND	ND	ND	4/24/84
82-65	1 - WN - SV - 45+	22.5	1.326	.247	.011	5/10/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/13/84
82-72	2 - SA - SV - 45+	26.1	1.328	.120	.004	6/14/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/10/84

Appendix C-3

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 63-25-2

Data Report - Carbaryl

Fraction: 15/50% SMV

RRf: 0.212

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	ND	ND	ND	4/26/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/14/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/24/84
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/24/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/25/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/10/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	5/14/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/14/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	ND	ND	ND	4/27/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/18/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/18/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/16/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/13/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/13/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/9/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/15/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/14/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/25/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/11/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/26/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/14/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/24/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/16/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/25/84
82-57	1 - EN - SV - 45+	19.8	ND	ND	ND	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/16/84
82-62	3 - EN - SV - 45+	23.2	ND	ND	ND	6/16/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/15/84
82-60	2 - EN - SV - 45+	26.2	ND	ND	ND	6/14/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/14/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/14/84
82-69	1 - SA - SV - 45+	20.0	1.081	46.501	2.325	4/24/84
82-65	1 - WN - SV - 45+	22.5	ND	ND	ND	5/10/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/13/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/14/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/10/84

Appendix C-4

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 95-48-7

Data Report - o-Cresol (o-methylphenol)

Fraction: 15/50% SMV

RRf: 0.651

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	.373	.954	.046	4/26/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/14/84
82-46	1 - PA - SV - 0-14	19.7	.369	.329	.016	4/24/84
82-36	1 - MO - SV - 0-14	9.0	.364	.471	.052	4/24/84
82-42	1 - NE - SV - 0-14	19.1	.365	.117	.006	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - BN - SV - 0-14	18.1	.360	.240	.013	4/25/84
82-63	1 - WN - SV - 0-14	23.4	.373	.235	.010	5/10/84
82-77	1 - ES - SV - 0-14	28.1	.353	1.255	.044	5/14/84
82-52	2 - MA - SV - 0-14	20.2	.335	5.870	.290	6/13/84
82-70	2 - SA - SV - 0-14	19.1	.338	1.155	.060	6/14/84
82-58	2 - BN - SV - 0-14	21.2	.341	1.799	.084	6/14/84
82-43	1 - NE - SV - 15-44	21.9	.340	.316	.014	4/15/84
82-50	1 - MA - SV - 15-44	25.2	.336	.262	.010	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	ND	ND	ND	4/27/84
82-61	3 - BN - SV - 15-44	20.2	ND	ND	ND	6/18/84
82-75	4 - SA - SV - 15-44	18.2	.327	.150	.008	6/18/84
82-73	3 - SA - SV - 15-44	17.9	.296	.049	.002	6/16/84
82-71	2 - SA - SV - 15-44	19.5	.341	.348	.017	6/13/84
82-53	2 - MA - SV - 15-44	26.1	.329	3.374	.129	6/13/84
82-83	1 - WS - SV - 15-44	22.7	.374	.615	.027	5/9/84
82-85	2 - WS - SV - 15-44	21.9	.330	1.313	.059	6/15/84
82-59	2 - BN - SV - 15-44	21.4	.339	.682	.031	6/14/84
82-37	1 - MO - SV - 15-44	18.3	.354	.474	.025	4/25/84
82-64	1 - WN - SV - 15-44	20.6	.359	.970	.047	5/11/84
82-56	1 - BN - SV - 15-44	21.6	.368	.295	.013	4/26/84
82-78	1 - ES - SV - 15-44	19.9	.346	.894	.044	5/14/84
82-68	1 - SA - SV - 15-44	26.4	.356	.319	.012	4/24/84
82-51	1 - MA - SV - 45+	16.2	.348	.296	.018	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	.297	.002	<.001	6/16/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/25/84
82-57	1 - BN - SV - 45+	19.8	.366	.112	.005	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	.291	.044	.002	6/16/84
82-62	3 - BN - SV - 45+	23.2	.291	.059	.002	6/16/84
82-66	2 - WN - SV - 45+	21.4	.335	2.478	.115	6/15/84
82-60	2 - BN - SV - 45+	26.2	.345	.285	.010	6/14/84
82-41	1 - MO - SV - 45+	21.0	.351	.720	.034	5/14/84
82-79	1 - ES - SV - 45+	20.7	.371	.906	.043	5/14/84
82-69	1 - SA - SV - 45+	20.0	.361	.272	.013	4/24/84
82-65	1 - WN - SV - 45+	22.5	.375	.329	.014	5/10/84
82-54	2 - MA - SV - 45+	18.1	.333	1.329	.073	6/13/84
82-72	2 - SA - SV - 45+	26.1	.398	.580	.022	6/14/84
82-84	1 - WS - SV - 45+	22.4	.375	.226	.010	5/10/84

Appendix C-5

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 106-44-5

Data Report - m,p-Cresol (m,p-methylphenol)

Fraction: 15/50% SMV

RRf: 0.638

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	.403	.181	.008	4/26/84
82-82	1 - WS - SV - 0-14	11.1	.397	2.504	.225	5/14/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/24/84
82-36	1 - MO - SV - 0-14	9.0	.396	.077	.008	4/24/84
82-42	1 - NE - SV - 0-14	19.1	.391	.096	.005	4/23/84
82-49	1 - MA - SV - 0-14	23.0	.384	.133	.005	4/23/84
82-55	1 - EN - SV - 0-14	18.1	.392	.090	.004	4/25/84
82-63	1 - WN - SV - 0-14	23.4	.401	.301	.012	5/10/84
82-77	1 - ES - SV - 0-14	28.1	.382	1.017	.036	5/14/84
82-52	2 - MA - SV - 0-14	20.2	.371	1.719	.085	6/13/84
82-70	2 - SA - SV - 0-14	19.1	.374	.982	.051	6/14/84
82-58	2 - EN - SV - 0-14	21.2	.376	.995	.046	6/14/84
82-43	1 - NE - SV - 15-44	21.9	.375	.279	.012	4/15/84
82-50	1 - MA - SV - 15-44	25.2	.373	.155	.006	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	.382	.491	.022	4/27/84
82-61	3 - EN - SV - 15-44	20.2	.371	.138	.006	6/18/84
82-75	4 - SA - SV - 15-44	18.2	.365	.104	.005	6/18/84
82-73	3 - SA - SV - 15-44	17.9	.338	.026	.001	6/16/84
82-71	2 - SA - SV - 15-44	19.5	.378	.199	.010	6/13/84
82-53	2 - MA - SV - 15-44	26.1	.366	2.689	.103	6/13/84
82-83	1 - WS - SV - 15-44	22.7	.400	.261	.011	5/9/84
82-85	2 - WS - SV - 15-44	21.9	.366	2.098	.095	6/15/84
82-59	2 - EN - SV - 15-44	21.4	.373	.404	.018	6/14/84
82-37	1 - MO - SV - 15-44	18.3	.386	.113	.006	4/25/84
82-64	1 - WN - SV - 15-44	20.6	.379	1.618	.078	5/11/84
82-56	1 - EN - SV - 15-44	21.6	.401	.419	.019	4/26/84
82-78	1 - ES - SV - 15-44	19.9	.378	2.566	.128	5/14/84
82-68	1 - SA - SV - 15-44	26.4	.385	.369	.013	4/24/84
82-51	1 - MA - SV - 45+	16.2	.381	.191	.011	4/24/84
82-76	4 - SA - SV - 45+	17.6	.361	.304	.017	6/18/84
82-81	2 - ES - SV - 45+	21.1	.336	.004	<.001	6/16/84
82-48	1 - PA - SV - 45+	22.0	.386	.412	.018	4/25/84
82-57	1 - EN - SV - 45+	19.8	.398	.422	.021	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	.332	.571	.031	6/16/84
82-62	3 - EN - SV - 45+	23.2	.332	.382	.016	6/16/84
82-66	2 - WN - SV - 45+	21.4	.368	9.356	.437	6/15/84
82-60	2 - EN - SV - 45+	26.2	.380	.449	.017	6/14/84
82-41	1 - MO - SV - 45+	21.0	.385	1.615	.076	5/14/84
82-79	1 - ES - SV - 45+	20.7	.399	.457	.022	5/14/84
82-69	1 - SA - SV - 45+	20.0	.393	.158	.007	4/24/84
82-65	1 - WN - SV - 45+	22.5	.400	.352	.015	5/10/84
82-54	2 - MA - SV - 45+	18.1	.367	.792	.043	6/13/84
82-72	2 - SA - SV - 45+	26.1	.428	1.114	.042	6/14/84
82-84	1 - WS - SV - 45+	22.4	.402	.117	.005	5/10/84

Appendix C-6

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 117-81-7

Data Report - Di-(2-ethylhexyl)phthalate (DEHP) Fraction: 15/50% SMV

RRf: 0.898

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	1.445	3.549	.171	4/26/84
82-82	1 - WS - SV - 0-14	11.1	1.457	4.738	.426	5/14/84
82-46	1 - PA - SV - 0-14	19.7	1.445	.830	.042	4/24/84
82-36	1 - MO - SV - 0-14	9.0	1.448	.391	.043	4/24/84
82-42	1 - NE - SV - 0-14	19.1	1.449	.141	.007	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - EN - SV - 0-14	18.1	1.449	.246	.013	4/25/84
82-63	1 - WN - SV - 0-14	23.4	1.452	1.989	.085	5/10/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	5/14/84
82-52	2 - MA - SV - 0-14	20.2	1.464	2.740	.135	6/13/84
82-70	2 - SA - SV - 0-14	19.1	1.457	3.244	.169	6/14/84
82-58	2 - EN - SV - 0-14	21.2	1.464	19.963	.941	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	1.442	.325	.012	4/12/84
82-80	2 - ES - SV - 15-44	25.7	1.461	.222	.008	6/15/84
82-47	1 - PA - SV - 15-44	21.6	1.452	1.221	.056	4/27/84
82-61	3 - EN - SV - 15-44	20.2	1.460	.297	.014	6/18/84
82-75	4 - SA - SV - 15-44	18.2	1.465	.305	.016	6/18/84
82-73	3 - SA - SV - 15-44	17.9	1.465	.292	.016	6/16/84
82-71	2 - SA - SV - 15-44	19.5	1.464	4.917	.252	6/13/84
82-53	2 - MA - SV - 15-44	26.1	1.465	17.965	.688	6/13/84
82-83	1 - WS - SV - 15-44	22.7	1.450	4.905	.216	5/9/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/15/84
82-59	2 - EN - SV - 15-44	21.4	1.465	2.807	.131	6/14/84
82-37	1 - MO - SV - 15-44	18.3	1.454	2.369	.129	4/25/84
82-64	1 - WN - SV - 15-44	20.6	1.453	1.569	.076	5/11/84
82-56	1 - EN - SV - 15-44	21.6	1.443	.337	.015	4/26/84
82-78	1 - ES - SV - 15-44	19.9	1.456	5.228	.262	5/14/84
82-68	1 - SA - SV - 15-44	26.4	1.451	2.939	.111	4/24/84
82-51	1 - MA - SV - 45+	16.2	1.453	.076	.004	4/24/84
82-76	4 - SA - SV - 45+	17.6	1.463	.053	.003	6/18/84
82-81	2 - ES - SV - 45+	21.1	1.459	.012	<.001	6/16/84
82-48	1 - PA - SV - 45+	22.0	1.451	2.835	.128	4/25/84
82-57	1 - EN - SV - 45+	19.8	1.446	.445	.022	4/26/84
82-44	1 - NE - SV - 45+	26.7	1.451	.050	.001	4/23/84
82-74	3 - SA - SV - 45+	18.0	1.464	.445	.024	6/16/84
82-62	3 - EN - SV - 45+	23.2	1.464	.654	.028	6/16/84
82-66	2 - WN - SV - 45+	21.4	1.462	2.493	.116	6/15/84
82-60	2 - EN - SV - 45+	26.2	1.459	4.871	.185	6/14/84
82-41	1 - MO - SV - 45+	21.0	1.457	2.424	.115	5/14/84
82-79	1 - ES - SV - 45+	20.7	1.456	8.009	.386	5/14/84
82-69	1 - SA - SV - 45+	20.0	1.447	1.081	.054	4/24/84
82-65	1 - WN - SV - 45+	22.5	1.453	3.278	.145	5/10/84
82-54	2 - MA - SV - 45+	18.1	1.464	3.822	.211	6/13/84
82-72	2 - SA - SV - 45+	26.1	1.455	5.187	.198	6/14/84
82-84	1 - WS - SV - 45+	22.4	1.456	.700	.031	5/10/84

Appendix C-7

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 95-80-7

Data Report - 2,4-Diaminotoluene

Fraction: 15/50% SMV

RRf: 0.581

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	ND	ND	ND	4/26/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/14/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/24/84
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/24/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/25/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/10/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	5/14/84
82-52	2 - MA - SV - 0-14	20.2	.658	3.261	.161	6/13/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/14/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	ND	ND	ND	4/27/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/18/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/18/84
82-73	3 - SA - SV - 15-44	17.9	.651	.039	.002	6/16/84
82-71	2 - SA - SV - 15-44	19.5	.658	.630	.032	6/13/84
82-53	2 - MA - SV - 15-44	26.1	.653	3.593	.137	6/13/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/9/84
82-85	2 - WS - SV - 15-44	21.9	.649	5.225	.238	6/15/84
82-59	2 - EN - SV - 15-44	21.4	.653	1.822	.085	6/14/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/25/84
82-64	1 - WN - SV - 15-44	20.6	.651	1.277	.062	5/11/84
82-56	1 - EN - SV - 15-44	21.6	.658	.438	.020	4/26/84
82-78	1 - ES - SV - 15-44	19.9	.651	2.605	.130	5/14/84
82-68	1 - SA - SV - 15-44	26.4	.785	.527	.019	4/24/84
82-51	1 - MA - SV - 45+	16.2	.646	.530	.032	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/16/84
82-48	1 - PA - SV - 45+	22.0	.649	.153	.006	4/25/84
82-57	1 - EN - SV - 45+	19.8	.657	.192	.009	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	.645	.123	.006	6/16/84
82-62	3 - EN - SV - 45+	23.2	ND	ND	ND	6/16/84
82-66	2 - WN - SV - 45+	21.4	.653	2.470	.115	6/15/84
82-60	2 - EN - SV - 45+	26.2	.657	.848	.032	6/14/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/14/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/14/84
82-69	1 - SA - SV - 45+	20.0	ND	ND	ND	4/24/84
82-65	1 - WN - SV - 45+	22.5	.653	1.630	.072	5/10/84
82-54	2 - MA - SV - 45+	18.1	.654	2.114	.116	6/13/84
82-72	2 - SA - SV - 45+	26.1	.665	3.480	.133	6/14/84
82-84	1 - WS - SV - 45+	22.4	.657	1.134	.050	5/10/84

Appendix C-8

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 613-69-4

Data Report - 2-Ethoxy benzaldehyde

Fraction: 15/50% SMV

RRf: 1.000

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	.623	.139	.006	4/26/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/14/84
82-46	1 - PA - SV - 0-14	19.7	.620	.036	.001	4/24/84
82-36	1 - MO - SV - 0-14	9.0	.616	.050	.005	4/24/84
82-42	1 - NE - SV - 0-14	19.1	ND	ND	ND	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/25/84
82-63	1 - WN - SV - 0-14	23.4	.615	.031	.001	5/10/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	5/14/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/14/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	ND	ND	ND	4/27/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/18/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/18/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/16/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/13/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/13/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/9/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/15/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/14/84
82-37	1 - MO - SV - 15-44	18.3	.611	.038	.002	4/25/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/11/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/26/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/14/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/24/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/16/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/25/84
82-57	1 - EN - SV - 45+	19.8	ND	ND	ND	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/16/84
82-62	3 - EN - SV - 45+	23.2	ND	ND	ND	6/16/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/15/84
82-60	2 - EN - SV - 45+	26.2	ND	ND	ND	6/14/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/14/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/14/84
82-69	1 - SA - SV - 45+	20.0	.617	.029	.001	4/24/84
82-65	1 - WN - SV - 45+	22.5	ND	ND	ND	5/10/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/13/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/14/84
82-84	1 - WS - SV - 45+	22.4	ND	ND	ND	5/10/84

Appendix C-9

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 6853-57-2

Data Report - 4-Pentyl benzaldehyde

Fraction: 15/50% SMV

RRf: 1.000

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	.742	.069	.003	4/26/84
82-82	1 - WS - SV - 0-14	11.1	ND	ND	ND	5/14/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/24/84
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/24/84
82-42	1 - NE - SV - 0-14	19.1	.737	.016	<.001	4/23/84
82-49	1 - MA - SV - 0-14	23.0	.737	.015	<.001	4/23/84
82-55	1 - EN - SV - 0-14	18.1	ND	ND	ND	4/25/84
82-63	1 - WN - SV - 0-14	23.4	.738	.067	.002	5/10/84
82-77	1 - ES - SV - 0-14	28.1	.734	.170	.006	5/14/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/14/84
82-58	2 - EN - SV - 0-14	21.2	ND	ND	ND	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	ND	ND	ND	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	ND	ND	ND	4/27/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/18/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/18/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/16/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/13/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/13/84
82-83	1 - WS - SV - 15-44	22.7	ND	ND	ND	5/9/84
82-85	2 - WS - SV - 15-44	21.9	ND	ND	ND	6/15/84
82-59	2 - EN - SV - 15-44	21.4	ND	ND	ND	6/14/84
82-37	1 - MO - SV - 15-44	18.3	ND	ND	ND	4/25/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/11/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/26/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/14/84
82-68	1 - SA - SV - 15-44	26.4	.736	.024	<.001	4/24/84
82-51	1 - MA - SV - 45+	16.2	ND	ND	ND	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/16/84
82-48	1 - PA - SV - 45+	22.0	ND	ND	ND	4/25/84
82-57	1 - EN - SV - 45+	19.8	ND	ND	ND	4/26/84
82-44	1 - NE - SV - 45+	26.7	ND	ND	ND	4/23/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/16/84
82-62	3 - EN - SV - 45+	23.2	ND	ND	ND	6/16/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/15/84
82-60	2 - EN - SV - 45+	26.2	ND	ND	ND	6/14/84
82-41	1 - MO - SV - 45+	21.0	ND	ND	ND	5/14/84
82-79	1 - ES - SV - 45+	20.7	.738	.138	.006	5/14/84
82-69	1 - SA - SV - 45+	20.0	.739	.040	.002	4/24/84
82-65	1 - WN - SV - 45+	22.5	ND	ND	ND	5/10/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/13/84
82-72	2 - SA - SV - 45+	26.1	ND	ND	ND	6/14/84
82-84	1 - WS - SV - 45+	22.4	.739	.043	.001	5/10/84

Appendix C-10

FY82 15/50% SMV Adipose Composite Summary

CAS No.: 90-43-7

Data Report - 2-Phenyl phenol (o-Phenol phenol) Fraction: 15/50% SMV

RRf: 0.333

MRI Sample Number	Sample Composite Number	Tissue Wt (g)	RRT	Amount (Total ug)	Concentration (ug/g)	Analysis Date
82-67	1 - SA - SV - 0-14	20.7	.790	.299	.014	4/26/84
82-82	1 - WS - SV - 0-14	11.1	.784	1.243	.112	5/14/84
82-46	1 - PA - SV - 0-14	19.7	ND	ND	ND	4/24/84
82-36	1 - MO - SV - 0-14	9.0	ND	ND	ND	4/24/84
82-42	1 - NE - SV - 0-14	19.1	.785	2.641	.138	4/23/84
82-49	1 - MA - SV - 0-14	23.0	ND	ND	ND	4/23/84
82-55	1 - EN - SV - 0-14	18.1	.787	1.867	.103	4/25/84
82-63	1 - WN - SV - 0-14	23.4	ND	ND	ND	5/10/84
82-77	1 - ES - SV - 0-14	28.1	ND	ND	ND	5/14/84
82-52	2 - MA - SV - 0-14	20.2	ND	ND	ND	6/13/84
82-70	2 - SA - SV - 0-14	19.1	ND	ND	ND	6/14/84
82-58	2 - EN - SV - 0-14	21.2	.782	1.121	.052	6/14/84
82-43	1 - NE - SV - 15-44	21.9	ND	ND	ND	4/15/84
82-50	1 - MA - SV - 15-44	25.2	.788	1.370	.054	4/12/84
82-80	2 - ES - SV - 15-44	25.7	ND	ND	ND	6/15/84
82-47	1 - PA - SV - 15-44	21.6	.785	.203	.009	4/27/84
82-61	3 - EN - SV - 15-44	20.2	ND	ND	ND	6/18/84
82-75	4 - SA - SV - 15-44	18.2	ND	ND	ND	6/18/84
82-73	3 - SA - SV - 15-44	17.9	ND	ND	ND	6/16/84
82-71	2 - SA - SV - 15-44	19.5	ND	ND	ND	6/13/84
82-53	2 - MA - SV - 15-44	26.1	ND	ND	ND	6/13/84
82-83	1 - WS - SV - 15-44	22.7	.788	5.808	.255	5/9/84
82-85	2 - WS - SV - 15-44	21.9	.779	7.155	.326	6/15/84
82-59	2 - EN - SV - 15-44	21.4	.781	.461	.021	6/14/84
82-37	1 - MO - SV - 15-44	18.3	.785	.900	.049	4/25/84
82-64	1 - WN - SV - 15-44	20.6	ND	ND	ND	5/11/84
82-56	1 - EN - SV - 15-44	21.6	ND	ND	ND	4/26/84
82-78	1 - ES - SV - 15-44	19.9	ND	ND	ND	5/14/84
82-68	1 - SA - SV - 15-44	26.4	ND	ND	ND	4/24/84
82-51	1 - MA - SV - 45+	16.2	.783	1.244	.076	4/24/84
82-76	4 - SA - SV - 45+	17.6	ND	ND	ND	6/18/84
82-81	2 - ES - SV - 45+	21.1	ND	ND	ND	6/16/84
82-48	1 - PA - SV - 45+	22.0	.785	.257	.011	4/25/84
82-57	1 - EN - SV - 45+	19.8	.790	.286	.014	4/26/84
82-44	1 - NE - SV - 45+	26.7	.784	9.366	.350	4/23/84
82-74	3 - SA - SV - 45+	18.0	ND	ND	ND	6/16/84
82-62	3 - EN - SV - 45+	23.2	.777	.361	.015	6/16/84
82-66	2 - WN - SV - 45+	21.4	ND	ND	ND	6/15/84
82-60	2 - EN - SV - 45+	26.2	.783	.443	.016	6/14/84
82-41	1 - MO - SV - 45+	21.0	.783	23.087	1.099	5/14/84
82-79	1 - ES - SV - 45+	20.7	ND	ND	ND	5/14/84
82-69	1 - SA - SV - 45+	20.0	.787	1.042	.052	4/24/84
82-65	1 - WN - SV - 45+	22.5	.786	2.458	.109	5/10/84
82-54	2 - MA - SV - 45+	18.1	ND	ND	ND	6/13/84
82-72	2 - SA - SV - 45+	26.1	.787	1.018	.039	6/14/84
82-84	1 - WS - SV - 45+	22.4	.778	.445	.019	5/10/84

APPENDIX D

INCIDENCE OF VOA SARA/ECAD TARGET ANALYTES IN FY82 ADIPOSE COMPOSITES

Appendix D-1

Incidence of VOA SARA/ECAD Target Analytes in FY82 Adipose Composites

			NORTH-CENTRAL[a]								
			East North Central[b]						West North Central		
No.	Compound Name	CAS No	0-14 C		15-44			45+		0-14	15-44	45+
1	2-Amyl furan	3777-69-3	+	+[d]	+	+	+	+ - +		+	+	+
2	Bromoheptane	629-04-9	-	-	-	-	-	- - -		+	-	-
3	Bromopentane	110-53-2	-	-	-	-	-	- - -		+	-	-
4	Butyraldehyde	123-72-8	+	+	+	+	+	+ + +		+	+	+
5	Ethyl isovalerate	108-64-5	+	+	+	+	+	+ + +		+	+	+
6	1-Iodopentane	628-17-1	+	+	-	+	+	- - -		+	+	+
7	Isobutyraldehyde	78-84-2	+	+	+	+	+	+ + +		+	+	+
8	Limonene	138-86-3	+	+	+	+	+	+ - +		+	+	+
9	Nonenes (1-Nonene)	124-11-8	+	+	+	+	+	+ + +		+	+	+
10	3-Octen-2-one	1669-44-9	+	+	+	+	+	+ - +		+	+	+
11	Pentyl Alcohol (3-methyl-1-butanol)	123-51-3	+	+	+	+	+	- + +		+	+	+
12	Pentyl cyclohexane	4292-92-6	+	-	-	-	-	- - +		-	-	-
13	Trichloroethylene {Trichloroethene}	79-01-6	+	+	-	+	+	+ + +		-	-	+

Appendix D-2

Incidence of VOA SARA/ECAD Target Analytes in FY82 Adipose

			NORTHEAST[a]						
			New England[b]				Middle Atlantic		
No.	Compound Name	CAS No	0-14 C	15-44	45+		0-14	15-44	45+
1	2-Amyl furan	3777-69-3	+[d]	+	+		+	+	+
2	Bromoheptane	629-04-9	-	-	-		-	-	-
3	Bromopentane	110-53-2	-	-	-		-	-	-
4	Butyraldehyde	123-72-8	+	+	+		+	+	+
5	Ethyl isovalerate	108-64-5	+	+	+		+	+	+
6	1-Iodopentane	628-17-1	+	+	+		-	+	+
7	Isobutyraldehyde	78-84-2	+	+	+		+	+	+
8	Limonene	138-86-3	+	+	+		+	+	+
9	Nonenes (1-Nonene)	124-11-8	+	+	+		+	+	+
10	3-Octen-2-one	1669-44-9	+	+	+		+	+	+
11	Pentyl Alcohol (3-methyl-1-butanol)	123-51-3	-	+	-		+	+	+
12	Pentyl cyclohexane	4292-92-6	-	-	+		-	-	-
13	Trichloroethylene {Trichloroethene}	79-01-6	+	-	-		-	+	+

Notes:

a. Census region
b. Census division
c. Age group from which the composite samples were collected.
d. Pluses and minuses correspond to the the number of composites analyzed within a given census division. A "+" indicates that a compound was identified in a composite and a "-" indicates that the compound was not detected in a composite.

Appendix D-3

Incidence of VOA SARA/ECAD Target Analytes in FY82 Adipose

			SOUTH [a]								
			South Atlantic [b]			East S. Central			West S. Central		
No.	Compound Name	CAS No	0-14 [c]	15-44	45+	0-14	15-44	45+	0-14	15-44	45+
1	2-Amyl furan	3777-69-3	+ + [d]	+ + + +	+ + + +	+	+ +	+ +	+	+ +	+
2	Bromoheptane	629-04-9	- -	- - - -	- - - -	-	- -	+ -	-	+ -	-
3	Bromopentane	110-53-2	- -	- - - -	- - - -	-	- -	- -	-	+ -	-
4	Butyraldehyde	123-72-8	+ +	+ + + +	+ + + +	+	+ +	+ +	-	+ +	+
5	Ethyl isovalerate	108-64-5	+ +	+ + + +	+ + + +	+	+ +	- +	-	+ +	+
6	1-Iodopentane	628-17-1	- +	- + + -	+ + - +	+	- +	+ +	+	+ +	+
7	Isobutyraldehyde	78-84-2	+ +	+ + + +	+ - + +	+	- +	+ +	-	+ +	+
8	Limonene	138-86-3	+ +	+ + + +	+ + + +	+	+ +	+ +	+	+ +	+
9	Nonenes (1-Nonene)	124-11-8	+ +	+ + + +	+ + + +	+	+ +	+ +	+	+ +	+
10	3-Octen-2-one	1669-44-9	+ +	+ + + +	+ + + +	+	+ +	+ +	+	+ +	+
11	Pentyl Alcohol (3-methyl-1-butanol)	123-51-3	- -	+ + + +	+ + + +	+	+ +	+ +	-	- +	+
12	Pentyl cyclohexane	4292-92-6	- -	+ - + +	- + + -	-	- +	- -	-	- +	-
13	Trichloroethylene {Trichloroethene}	79-01-6	- -	- - + -	+ - - -	-	- +	- +	-	- +	-

Appendix D-4

Incidence of VOA SARA/ECAD Target Analytes in FY82 Adipose

			WEST [a]					
			Mountain [b]			Pacific		
No.	Compound Name	CAS No	0-14 [c]	15-44	45+	0-14	15-44	45+
1	2-Amyl furan	3777-69-3	+ [d]	+	+	+	+	+
2	Bromoheptane	629-04-9	-	-	-	+	-	-
3	Bromopentane	110-53-2	-	-	-	+	-	-
4	Butyraldehyde	123-72-8	+	+	+	+	+	+
5	Ethyl isovalerate	108-64-5	+	+	+	+	+	+
6	1-Iodopentane	628-17-1	+	+	-	+	+	+
7	Isobutyraldehyde	78-84-2	+	+	+	+	+	+
8	Limonene	138-86-3	+	+	+	+	+	+
9	Nonenes (1-Nonene)	124-11-8	+	+	+	+	+	+
10	3-Octen-2-one	1669-44-9	+	+	+	+	+	+
11	Pentyl Alcohol (3-methyl-1-butanol)	123-51-3	-	-	+	+	+	+
12	Pentyl cyclohexane	4292-92-6	-	-	-	-	-	-
13	Trichloroethylene {Trichloroethene}	79-01-6	-	-	-	-	+	+

Notes:

a. Census region
b. Census division
c. Age group from which the composite samples were collected.
d. Pluses and minuses correspond to the the number of composites analyzed within a given census division. A "+" indicates that a compound was identified in a composite and a "-" indicates that the compound was not detected in a composite.

APPENDIX E

INCIDENCE OF 6% SMV SARA/ECAD TARGET ANALYTES IN FY82 ADIPOSE

Appendix E-1

Incidence of 6% SMV SARA/ECAD Target Analytes in FY82 Adipose

No.	Compound Name	CAS No	NORTH CENTRAL[a]					
			East North Central[b]			West North Central		
			0-14[c]	15-44	45+	0-14	15-44	45+
1	Anthracene	120-12-7	- -[d]	- - -	- - -	-	-	-
2	Biphenyl	92-52-4	- -	- - -	- - -	+	-	+
3	Cymene (isopropyltoluene)	99-87-6	+ -	+ + +	+ + +	+	+	+
4	Dibenzofuran	132-64-9	- -	- - -	- - -	-	-	-
5	Diphenyl ether (1,1'-Oxybisbenzene)	101-84-8	+ +	+ + +	+ + +	+	+	+
6	Limonene	138-86-3	+ -	+ + +	+ + +	+	+	+
7	Safrole	94-59-7	- -	- - -	- - -	-	-	-
8	1,2,4-Trimethylbenzene	95-63-6	+ -	+ + +	+ + +	+	+	+
9	2,6-Xylidine	87-62-7	- -	- - -	+ + +	-	-	+

Appendix E-2

Incidence of 6% SMV SARA/ECAD Target Analytes in FY82

No.	Compound Name	CAS No	NORTHEAST[a]					
			New England[b]			Middle Atlantic		
			0-14[c]	15-44	45+	0-14	15-44	45+
1	Anthracene	120-12-7	-[d]	-	-	-	-	-
2	Biphenyl	92-52-4	-	-	-	-	-	-
3	Cymene (isopropyltoluene)	99-87-6	+	+	+	+	+	+
4	Dibenzofuran	132-64-9	-	-	-	-	+	-
5	Diphenyl ether (1,1'-Oxybisbenzene)	101-84-8	+	+	+	+	+	+
6	Limonene	138-86-3	+	+	+	+	+	+
7	Safrole	94-59-7	-	-	+	-	+	+
8	1,2,4-Trimethylbenzene	95-63-6	+	+	+	+	+	+
9	2,6-Xylidine	87-62-7	-	-	-	-	-	+

Notes:

a. Census region
b. Census division
c. Age group from which the composite samples were collected.
d. Pluses and minuses correspond to the the number of composites analyzed within a given census division. A "+" indicates that a compound was identified in a composite and a "-" indicates that the compound was not detected in a composite.

Appendix E-3

Incidence of 6% SMV SARA/ECAD Target Analytes in FY82 Adipose Composites

No.	Compound Name	CAS No	SOUTH [a]											
			South Atlantic [b]				East S. Central			West S. Central				
			0-14 [c]	15-44		45+	0-14	15-44	45+	0-14	15-44		45+	
1	Anthracene	120-12-7	- - [d]	- -	- -	- - - -	-	- -	- -	-	+	-	-	
2	Biphenyl	92-52-4	+ -	- -	- -	+ - - -	-	+ -	- +	-	+	-	-	
3	Cymene (isopropyltoluene)	99-87-6	+ +	+ +	+ +	+ + + -	+	+ -	- +	+	+	+	+	
4	Dibenzofuran	132-64-9	+ -	+ -	- -	- - - -	-	- -	- -	-	-	-	-	
5	Diphenyl ether (1,1'-Oxybisbenzene)	101-84-8	+ +	+ +	- +	+ + + +	+	+ -	- +	+	+	+	+	
6	Limonene	138-86-3	+ +	+ +	+ +	+ - + +	+	+ -	- +	+	+	+	+	
7	Safrole	94-59-7	- -	- -	- -	- - - -	-	- -	- -	-	-	-	-	
8	1,2,4-Trimethylbenzene	95-63-6	+ +	+ +	+ +	+ + + +	+	+ -	- +	+	+	+	+	
9	2,6-Xylidine	87-62-7	- -	- -	- -	+ - - +	-	+ -	- +	-	-	-	-	

Appendix E-4

Incidence of 6% SMV SARA/ECAD Target Analytes in FY82 Adipose Composites

No.	Compound Name	CAS No	WEST [a]					
			Mountain [b]			Pacific		
			0-14 [c]	15-44	45+	0-14	15-44	45+
1	Anthracene	120-12-7	- [d]	-	-	-	-	-
2	Biphenyl	92-52-4	-	-	+	-	-	+
3	Cymene (isopropyltoluene)	99-87-6	+	+	+	+	-	+
4	Dibenzofuran	132-64-9	-	-	-	-	-	-
5	Diphenyl ether (1,1'-Oxybisbenzene)	101-84-8	-	+	+	+	-	+
6	Limonene	138-86-3	+	+	+	+	-	+
7	Safrole	94-59-7	-	-	-	-	-	-
8	1,2,4-Trimethylbenzene	95-63-6	+	+	+	+	-	+
9	2,6-Xylidine	87-62-7	-	-	+	-	-	+

Notes:

a. Census region
b. Census division
c. Age group from which the composite samples were collected.
d. Pluses and minuses correspond to the the number of composites analyzed within a given census division. A "+" indicates that a compound was identified in a composite and a "-" indicates that the compound was not detected in a composite.

APPENDIX F

INCIDENCE OF 15/50% SMV SARA/ECAD TARGET ANALYTES IN FY82 COMPOSITES

Appendix F-1

Incidence of 15/50% SMV SARA/ECAD Target Analytes in FY82 Adipose

No.	Compound Name	CAS No	NORTH CENTRAL[a]								
			East North Central[b]						West North Central		
			0-14[c]	15-44		45+			0-14	15-44	45+
1	Bis(2-ethylhexyl)adipate	103-23-1	- -[d]	+ -	-	- -	-		-	-	-
2	Butyl glycol butyl phthalate	85-70-1	- -	- -	+	- +	+		-	+	+
3	Carbaryl	63-25-2	- -	- -	-	- -	-		-	-	-
4	o-Cresol (o-methylphenol)	95-48-7	+ +	+ +	-	+ +	+		+	+	+
5	m,p-Cresol (m,p-methylphenol)	106-44-5	+ +	+ +	+	+ +	+		+	+	+
6	Di-(2-ethylhexyl)phthalate (DEHP)	117-81-7	+ +	+ +	+	+ +	+		+	+	+
7	2,4-Diaminotoluene	95-80-7	- -	+ +	-	+ +	-		-	+	+
8	2-Ethoxy benzaldehyde	613-69-4	- -	- -	-	- -	-		+	-	-
9	4-Pentyl benzaldehyde	6853-57-2	- -	- -	-	- -	-		+	-	-
10	2-Phenyl phenol (o-Phenol phenol)	90-43-7	+ +	- +	-	+ +	+		-	-	+

Appendix F-2

Incidence of 15/50% SMV SARA/ECAD Target Analytes in FY82

No.	Compound Name	CAS No	NORTHEAST[a]					
			New England[b]			Middle Atlantic		
			0-14[c]	15-44	45+	0-14	15-44	45+
1	Bis(2-ethylhexyl)adipate	103-23-1	-[d]	-	-	-	+	-
2	Butyl glycol butyl phthalate	85-70-1	-	-	-	-	-	-
3	Carbaryl	63-25-2	-	-	-	-	-	-
4	o-Cresol (o-methylphenol)	95-48-7	+	+	-	+	+	+
5	m,p-Cresol (m,p-methylphenol)	106-44-5	+	+	-	+	+	+
6	Di-(2-ethylhexyl)phthalate (DEHP)	117-81-7	+	-	+	+	+	+
7	2,4-Diaminotoluene	95-80-7	-	-	-	+	+	+
8	2-Ethoxy benzaldehyde	613-69-4	-	-	-	-	-	-
9	4-Pentyl benzaldehyde	6853-57-2	+	-	-	+	-	-
10	2-Phenyl phenol (o-Phenol phenol)	90-43-7	+	-	+	-	+	+

Notes:

a. Census region

b. Census division

c. Age group from which the cmposite sample were collected.

d. Pluses and minuses correspond to the number of composites anlayzed within a given census division. A "+" indicates that a compound was identified in a composite and a "-" indicates that the compound was not detected in a composite.

Appendix F-3

Incidence of 15/50% SMV SARA/ECAD Target Analytes in FY82 Adipose Composites

No.	Compound Name	CAS No	SOUTH [a]											
			South Atlantic [b]				East S. Central			West S. Central				
			0-14 [c]	15-44		45+	0-14	15-44	45+	0-14	15-44	45+		
1	Bis(2-ethylhexyl)adipate	103-23-1	+ - [d]	- +	- -	+ +	- -	- -	+ -	-	- +	-
2	Butyl glycol butyl phthalate	85-70-1	- -	+ +	- -	- +	- -	- -	- -	-	- -	-
3	Carbaryl	63-25-2	- -	- -	- -	+ -	- -	- -	- -	-	- -	-
4	o-Cresol (o-methylphenol)	95-48-7	+ +	+ +	+ +	+ +	- +	+ -	+ +	-	+ +	+
5	m,p-Cresol (m,p-methylphenol)	106-44-5	+ +	+ +	+ +	+ +	+ +	+ -	+ +	+	+ +	+
6	Di-(2-ethylhexyl)phthalate (DEHP)	117-81-7	+ +	+ +	+ +	+ +	- +	+ +	+ +	+	+ -	+
7	2,4-Diaminotoluene	95-80-7	- -	+ +	+ -	- +	+ -	- -	- -	-	- +	+
8	2-Ethoxy benzaldehyde	613-69-4	+ -	- -	- -	+ -	- -	- -	- -	-	- -	-
9	4-Pentyl benzaldehyde	6853-57-2	+ -	+ -	- -	+ -	- +	- -	+ -	-	- -	+
10	2-Phenyl phenol (o-Phenol phenol)	90-43-7	+ -	- -	- -	+ +	- -	- -	- -	+	+ +	+

Appendix F-4

Incidence of 15/50% SMV SARA/ECAD Target Analytes in FY82 Adipose Composites

No.	Compound Name	CAS No	WEST [a]					
			Mountain [b]			Pacific		
			0-14 [c]	15-44	45+	0-14	15-44	45+
1	Bis(2-ethylhexyl)adipate	103-23-1	- [d]	-	-	-	-	-
2	Butyl glycol butyl phthalate	85-70-1	-	-	-	-	-	-
3	Carbaryl	63-25-2	-	-	-	-	-	-
4	o-Cresol (o-methylphenol)	95-48-7	+	+	+	+	-	-
5	m,p-Cresol (m,p-methylphenol)	106-44-5	+	+	+	-	+	+
6	Di-(2-ethylhexyl)phthalate (DEHP)	117-81-7	+	+	+	+	+	+
7	2,4-Diaminotoluene	95-80-7	-	-	-	-	-	+
8	2-Ethoxy benzaldehyde	613-69-4	+	+	-	+	-	-
9	4-Pentyl benzaldehyde	6853-57-2	-	-	-	-	-	-
10	2-Phenyl phenol (o-Phenol phenol)	90-43-7	-	+	+	-	+	+

Notes:

a. Census region

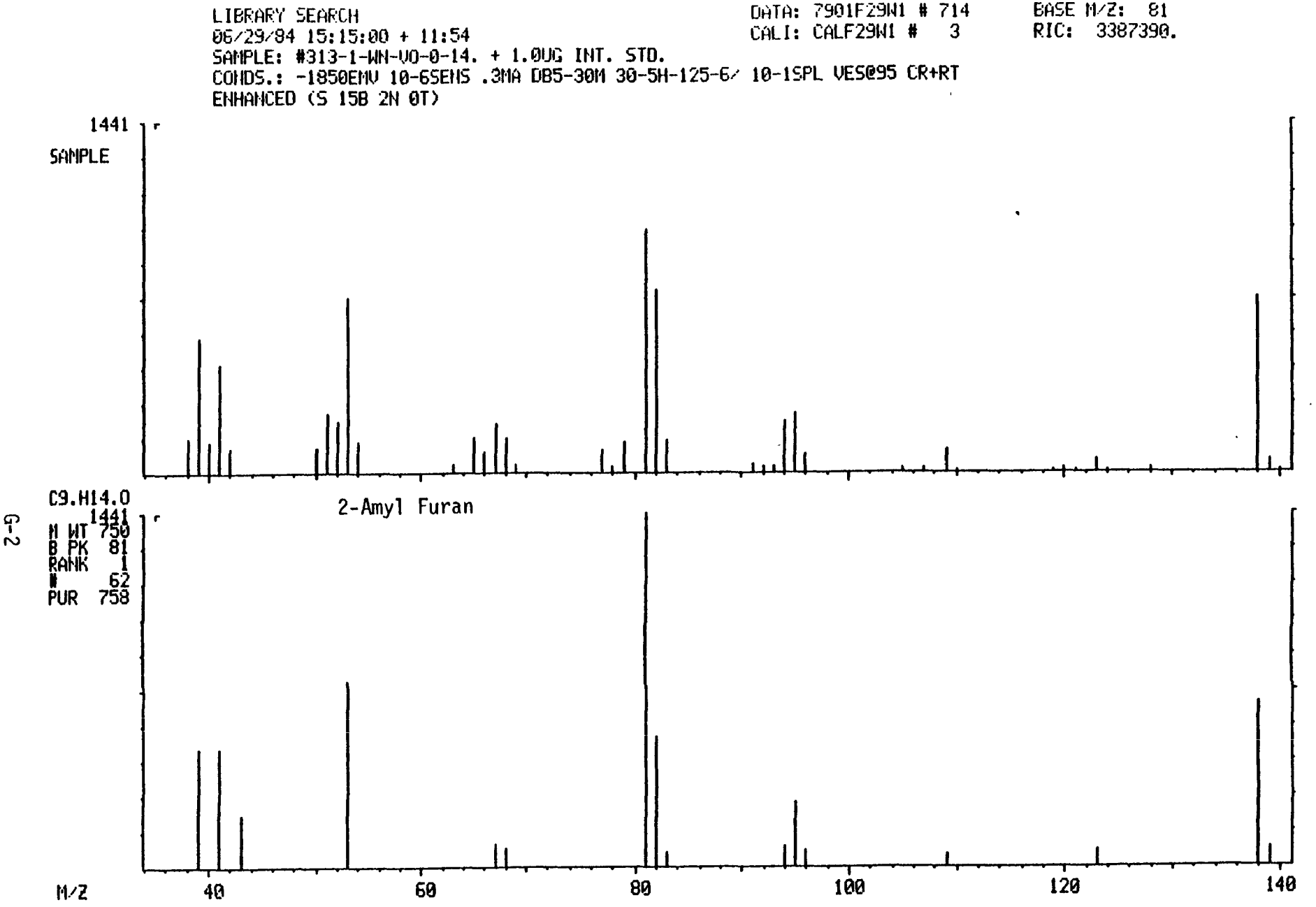
b. Census division

c. Age group from which the cmposite sample were collected.

d. Pluses and minuses correspond to the number of composites anlayzed within a given census division. A "+" indicates that a compound was identified in a composite and a "-" indicates that the compound was not detected in a composite.

APPENDIX G

COMPARISON PLOTS OF SAMPLE vs. REFERENCE MASS SPECTRA FOR COMPOUNDS IDENTIFIED IN FY82 COMPOSITES



G-2

Figure G-1. Mass spectral comparison of 2-amyl furan to a peak in NHATS volatile composite.

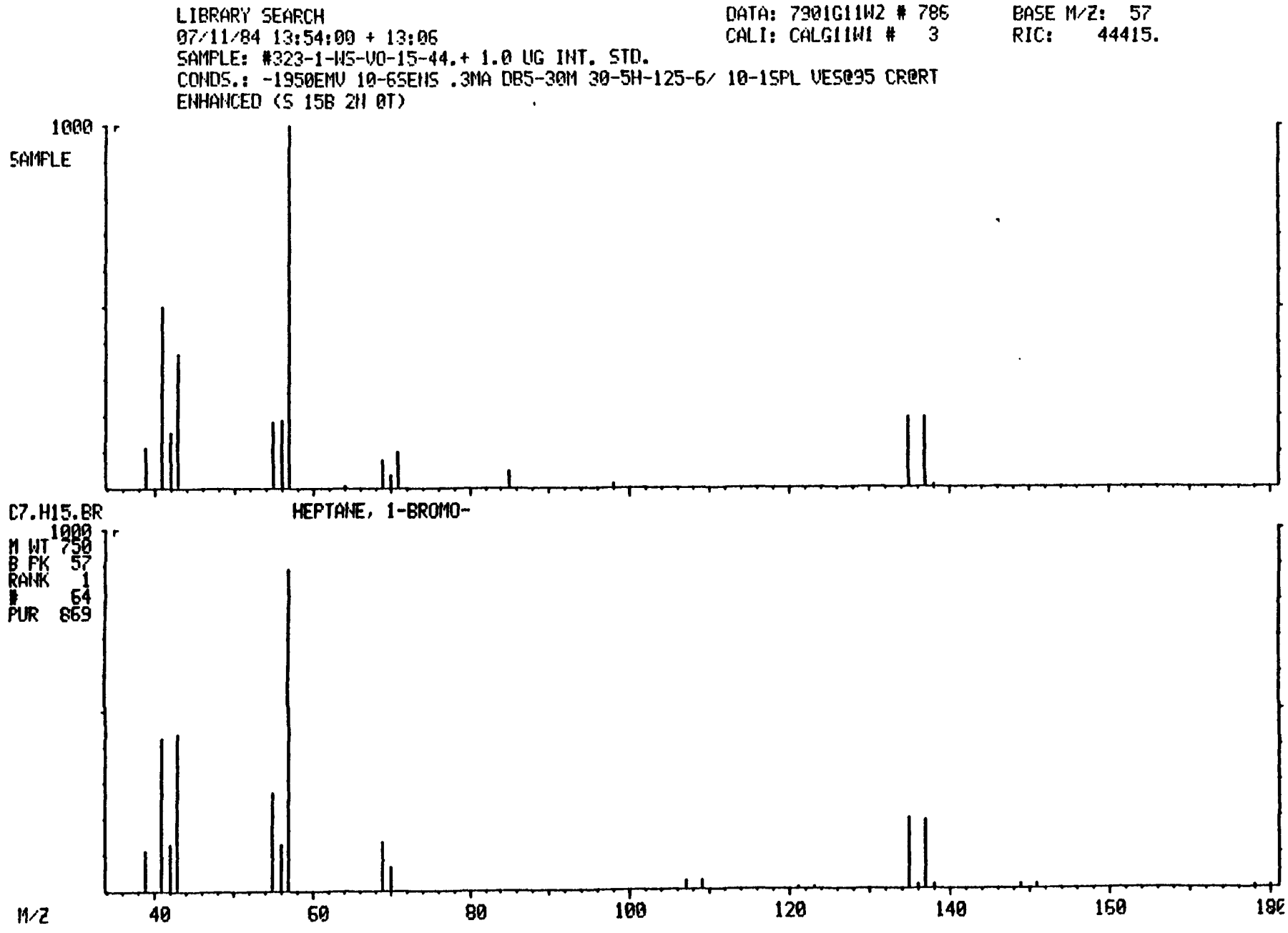


Figure G-2. Mass spectral comparison of 1-bromo-heptane to a peak in NHATS volatile composite.

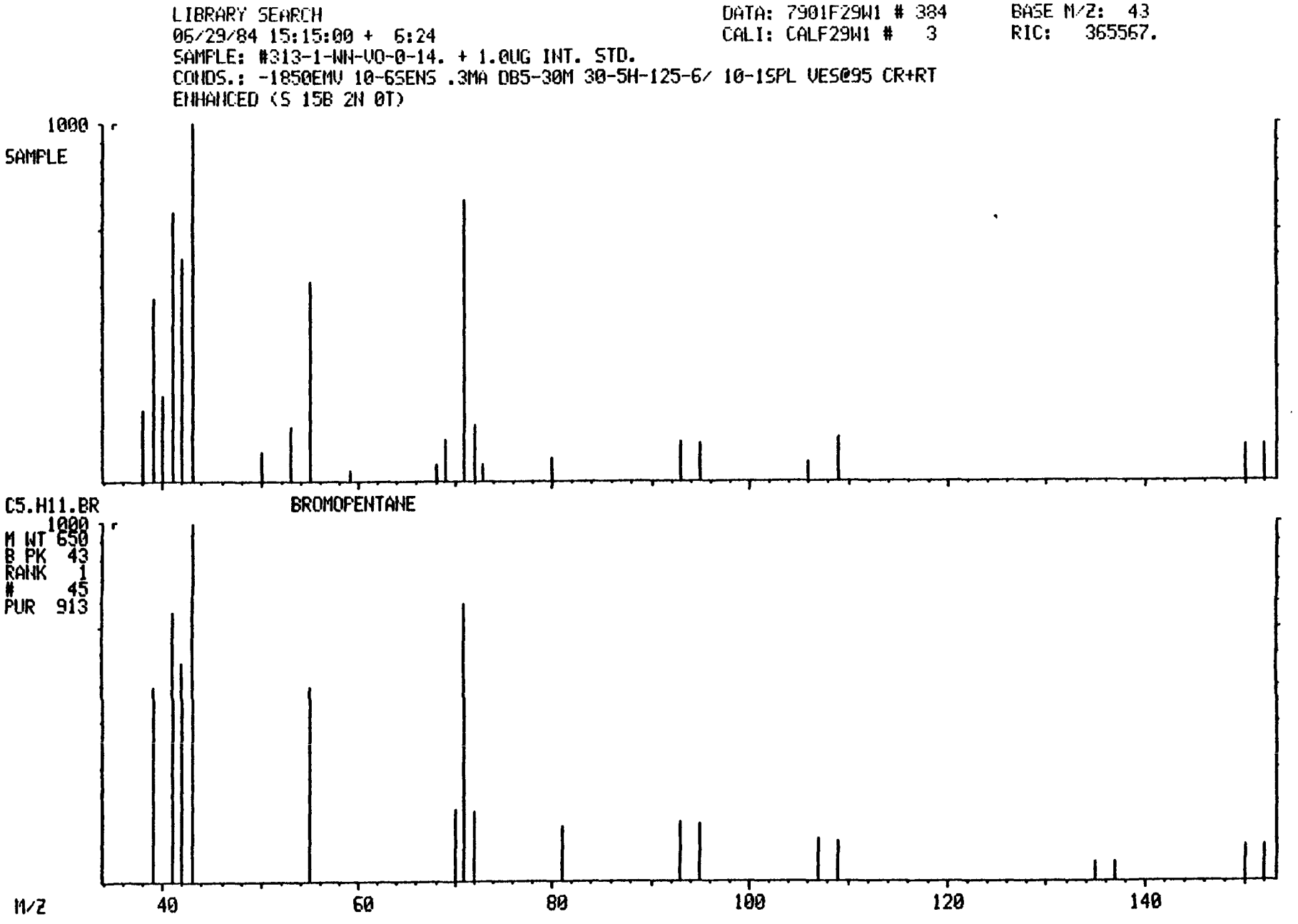


Figure G-3. Mass spectral comparison of bromopentane to a peak in NHATS volatile composite.

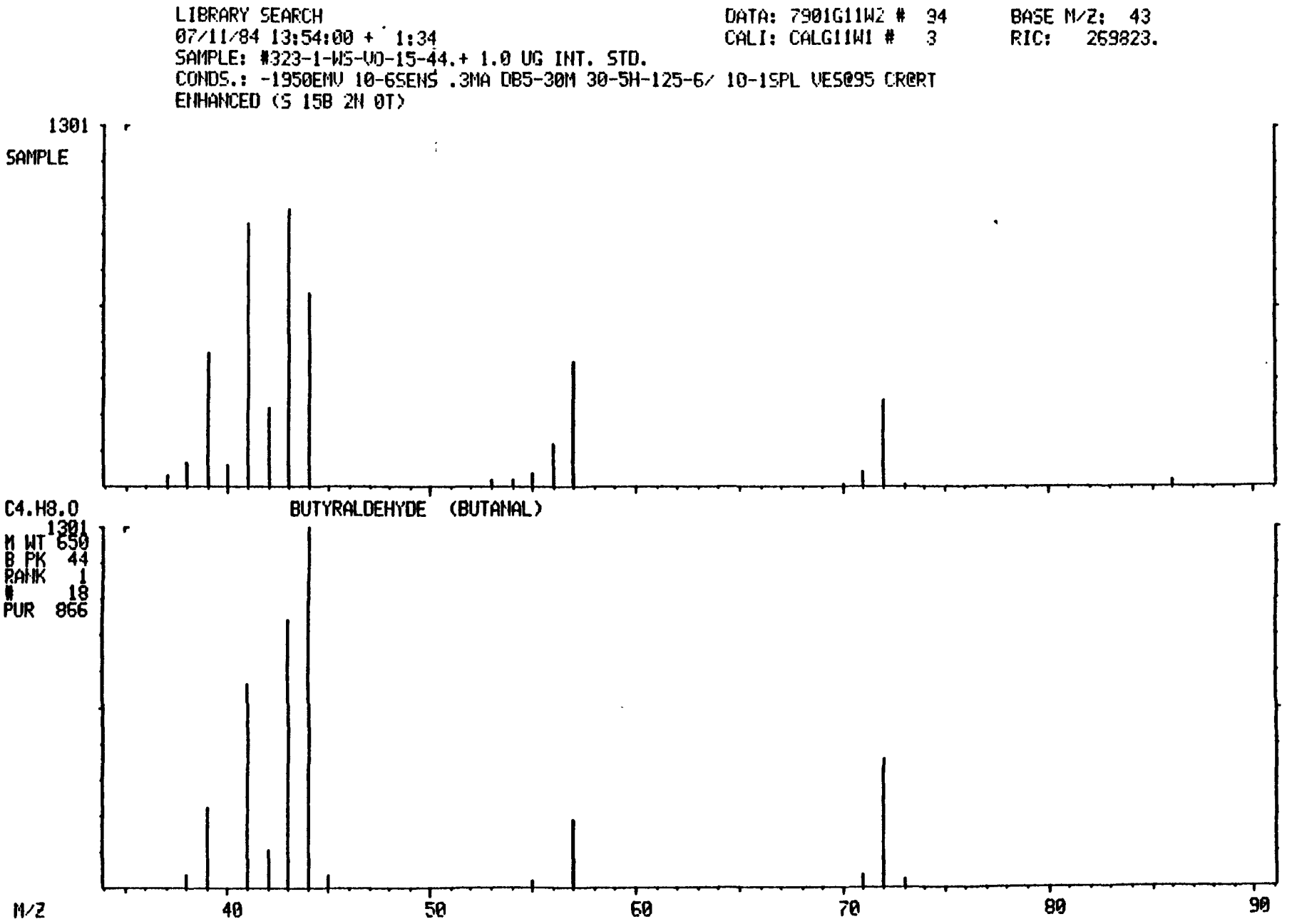


Figure G-4. Mass spectral comparison of butyraldehyde (butanal) to a peak in NHATS volatile composite.

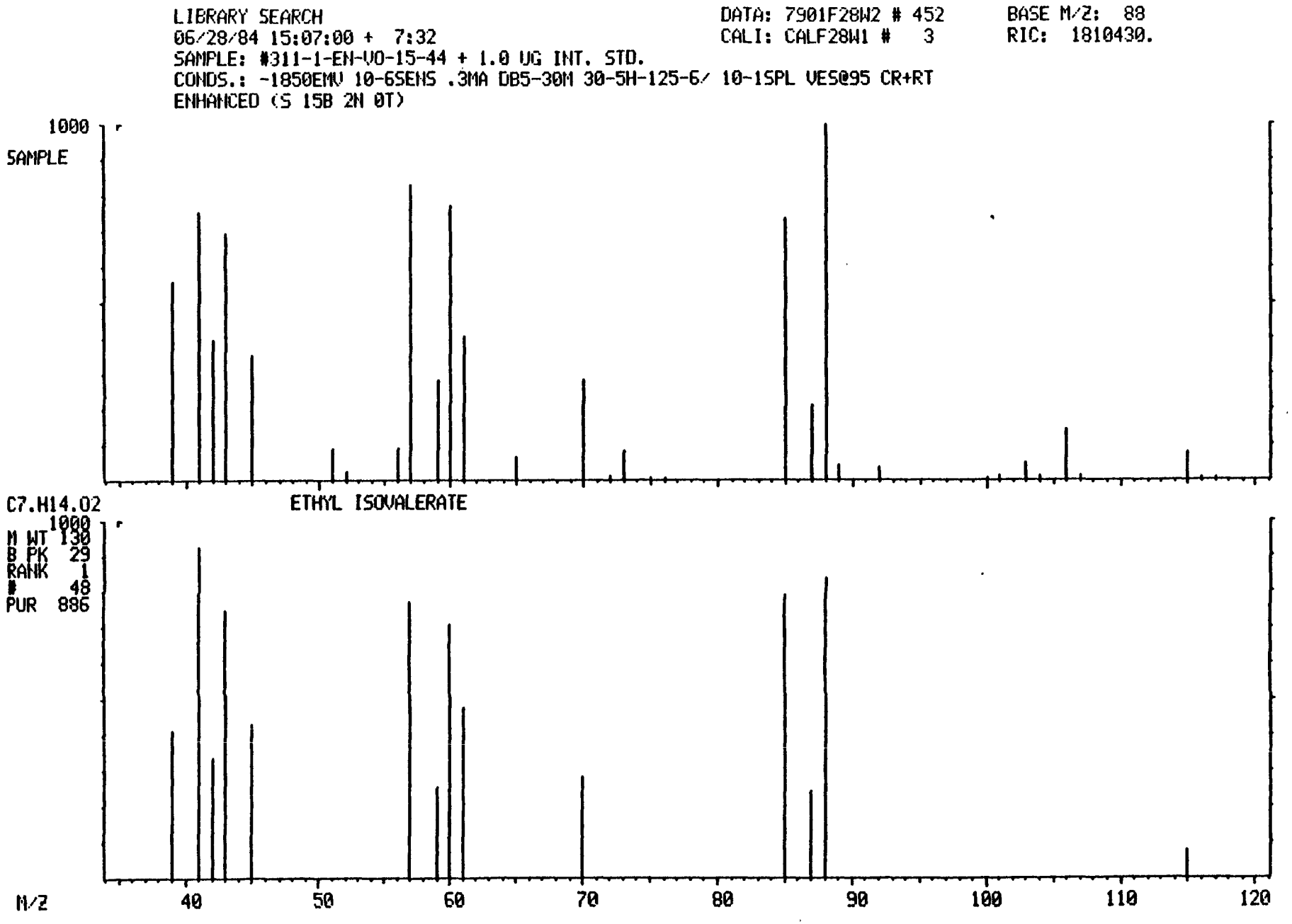


Figure G-5. Mass spectral comparison of ethyl isovalerate to a peak in NHATS volatile composite.

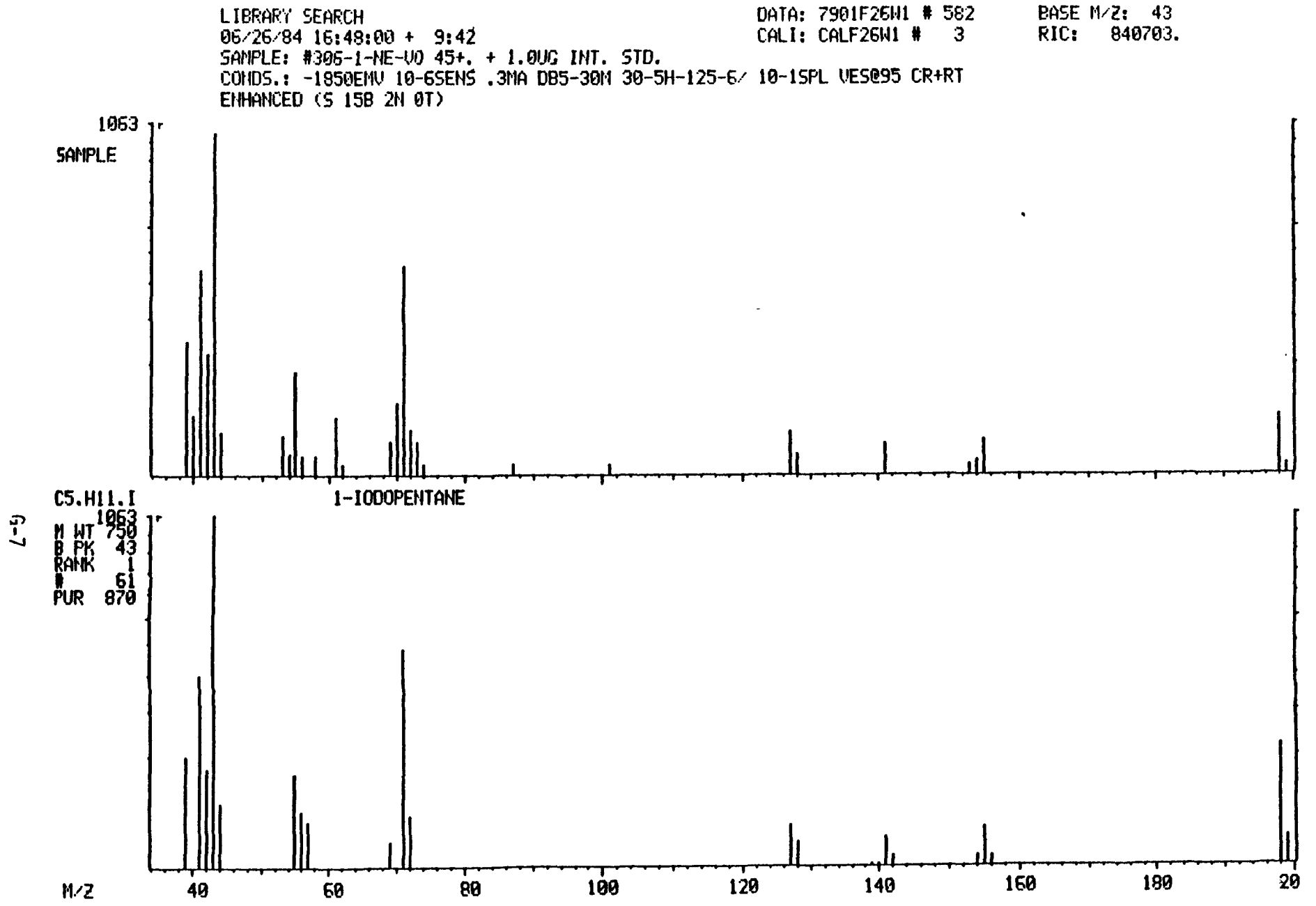


Figure G-6. Mass spectral comparison of 1-iodopentane to a peak in NHATS volatile composite.

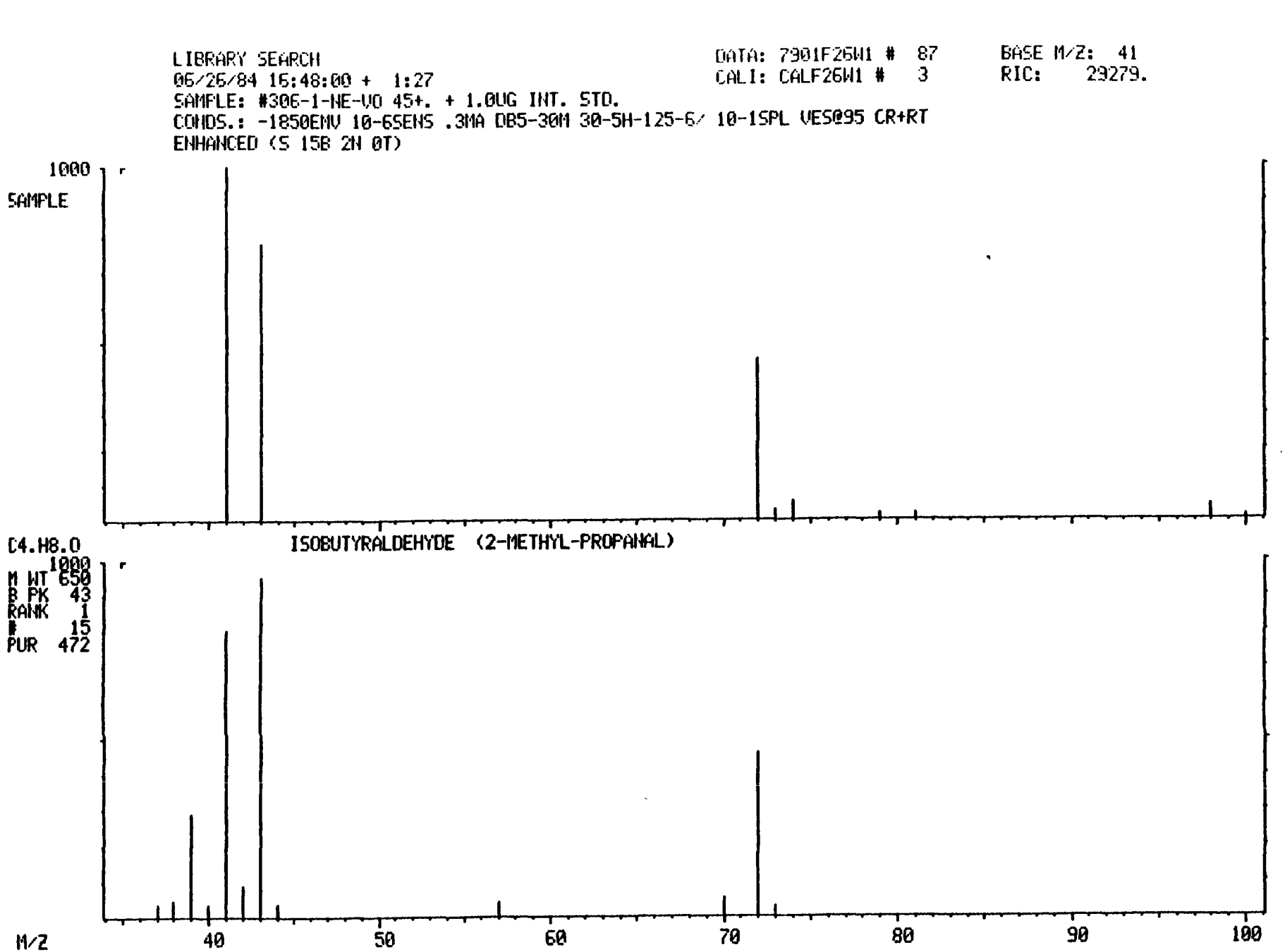


Figure G-7. Mass spectral comparison of isobutyraldehyde (2-methyl-propanal) to a peak in NHATS volatile composite.

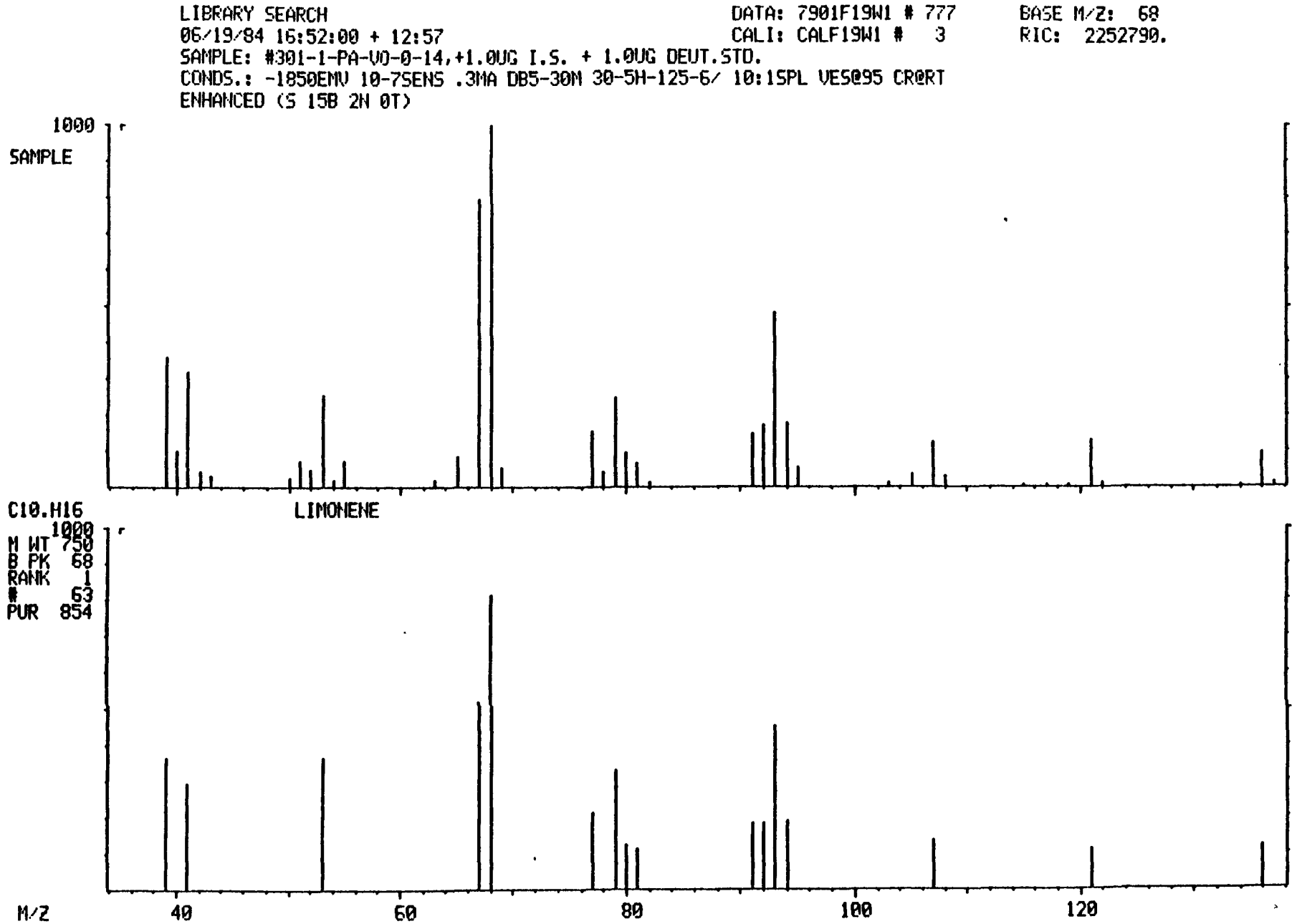


Figure G-8. Mass spectral comparison of limonene to a peak in NHATS volatile composite.

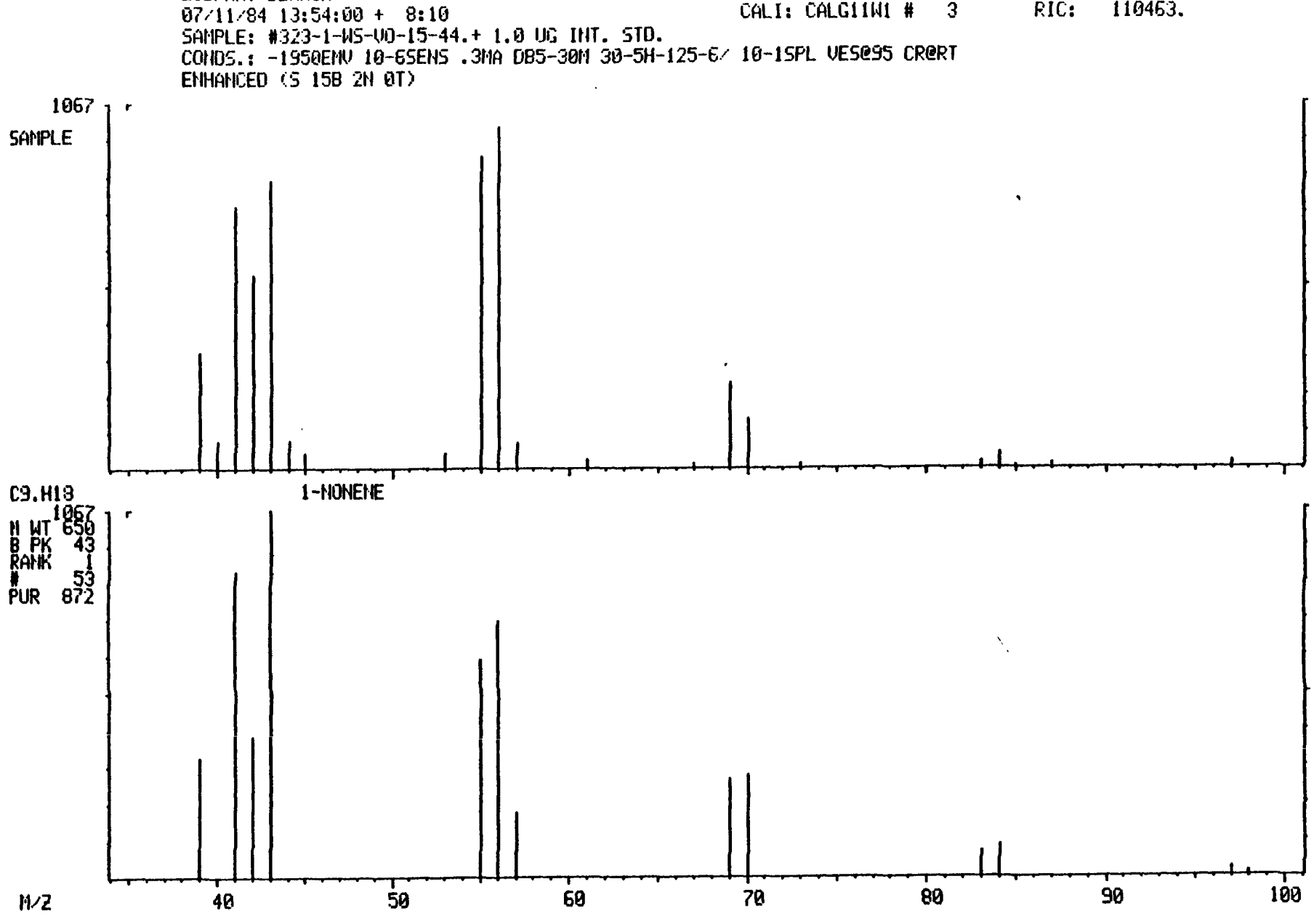


Figure G-9. Mass spectral comparison of 1-nonene to a peak in NHATS volatile composite.

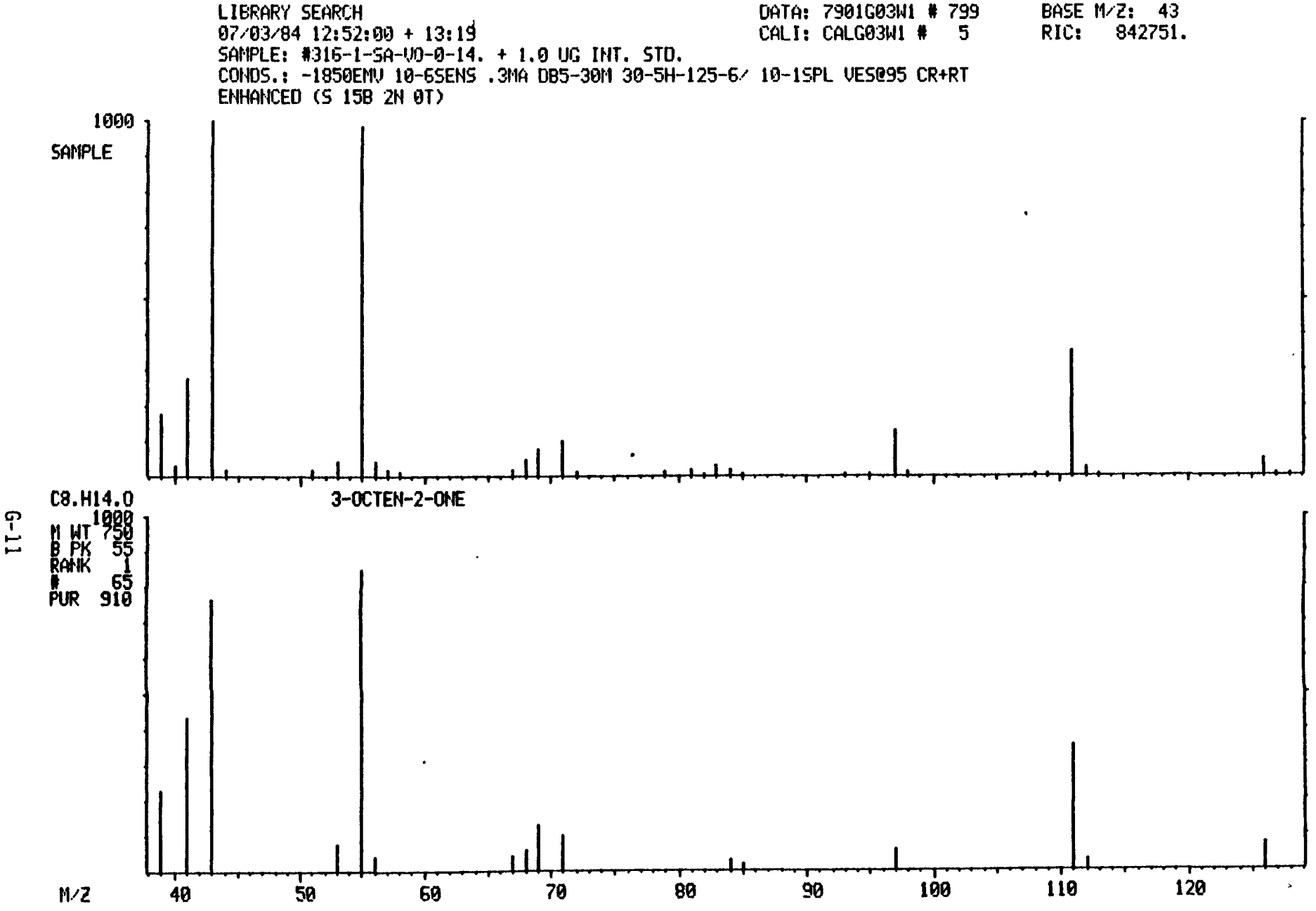


Figure G-10. Mass spectral comparison of 3-octen-2-one to a peak in NHATS volatile composite.

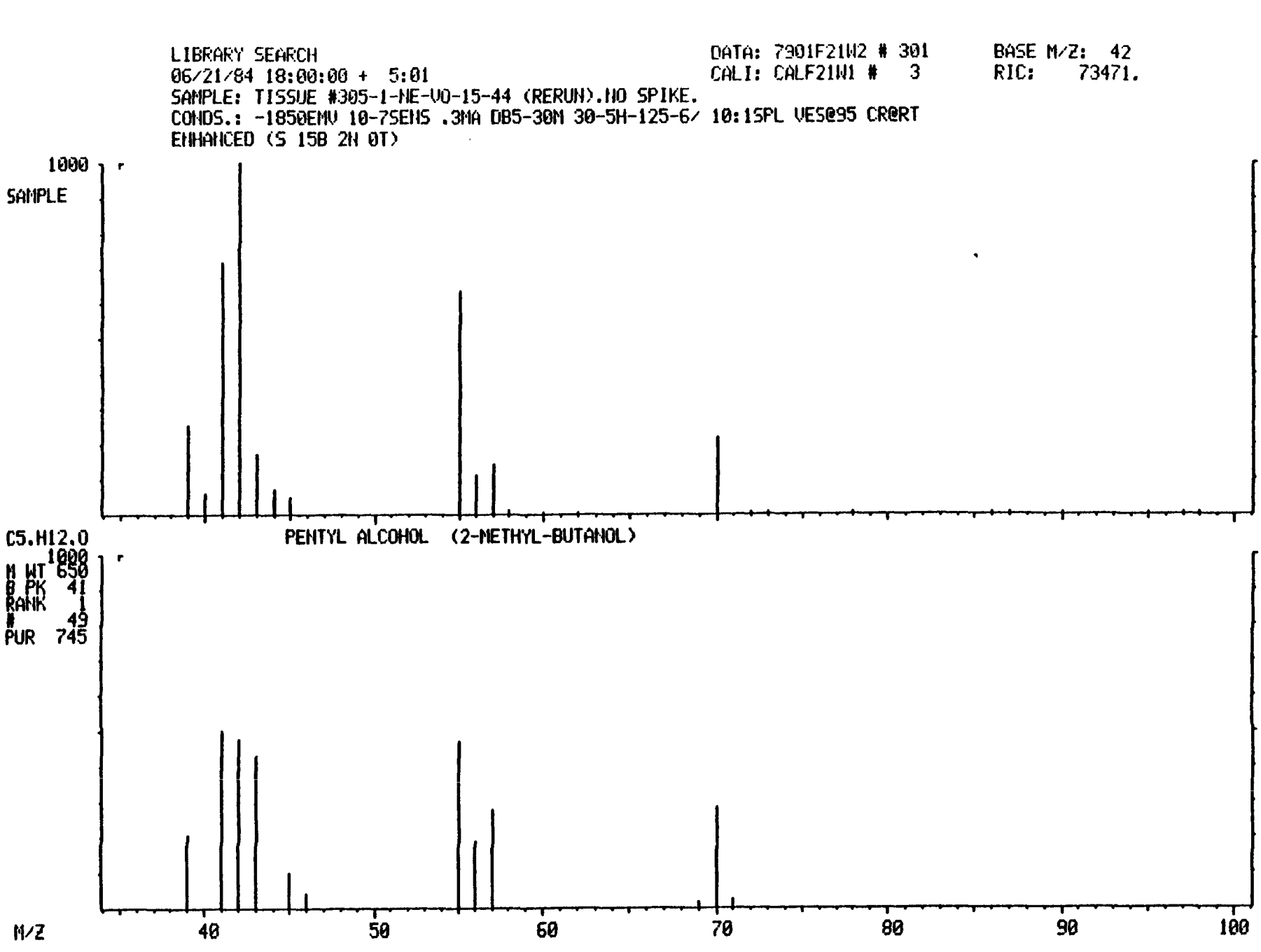


Figure G-11. Mass spectral comparison of pentyl alcohol (2-methyl-butanol) to a peak in NHATS volatile composite.

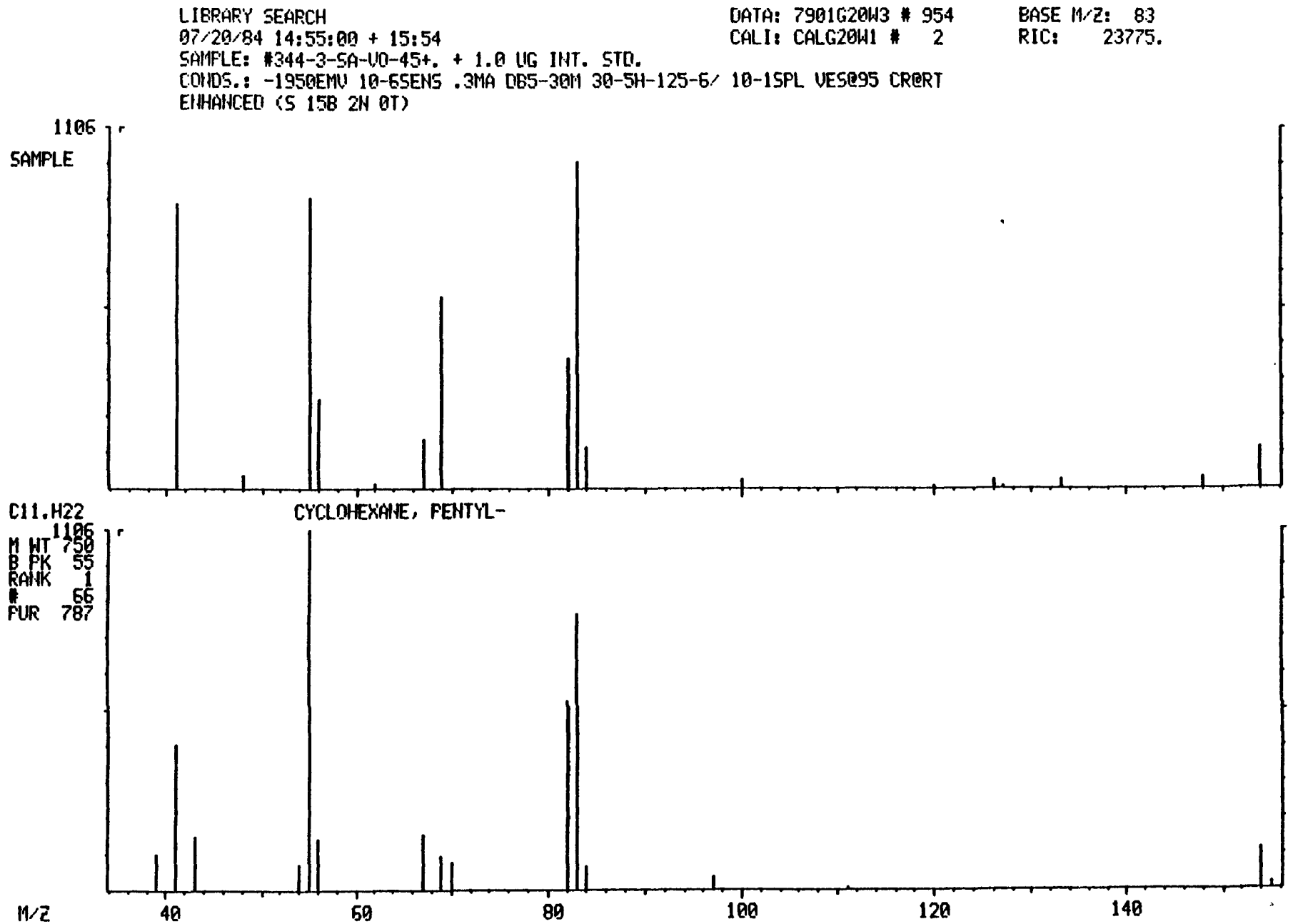


Figure G-12. Mass spectral comparison of pentyl cyclohexane to a peak in NHATS volatile composite.

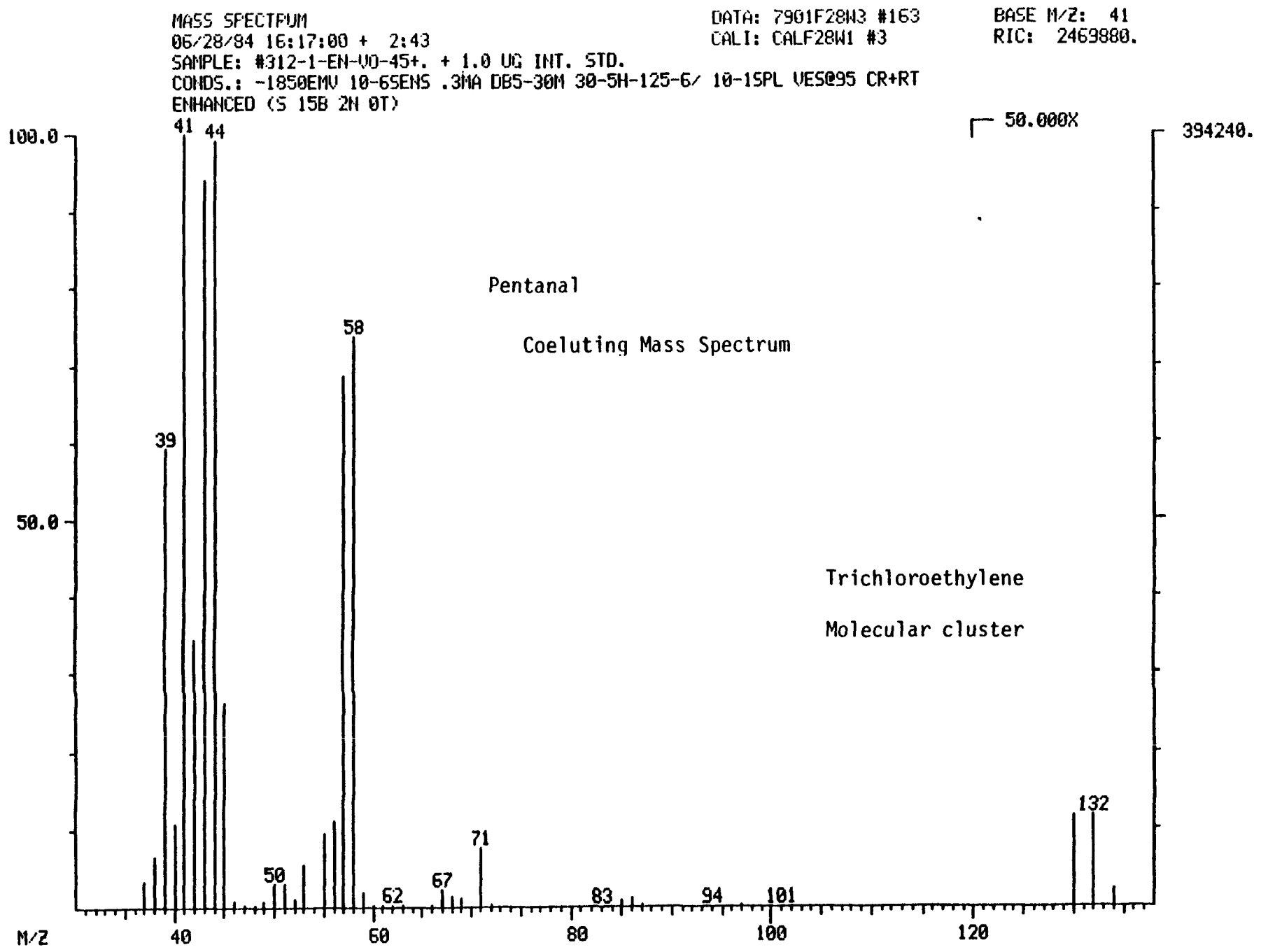


Figure G-13. Mass spectrum of trichloroethylene in presence of coeluting interferent.

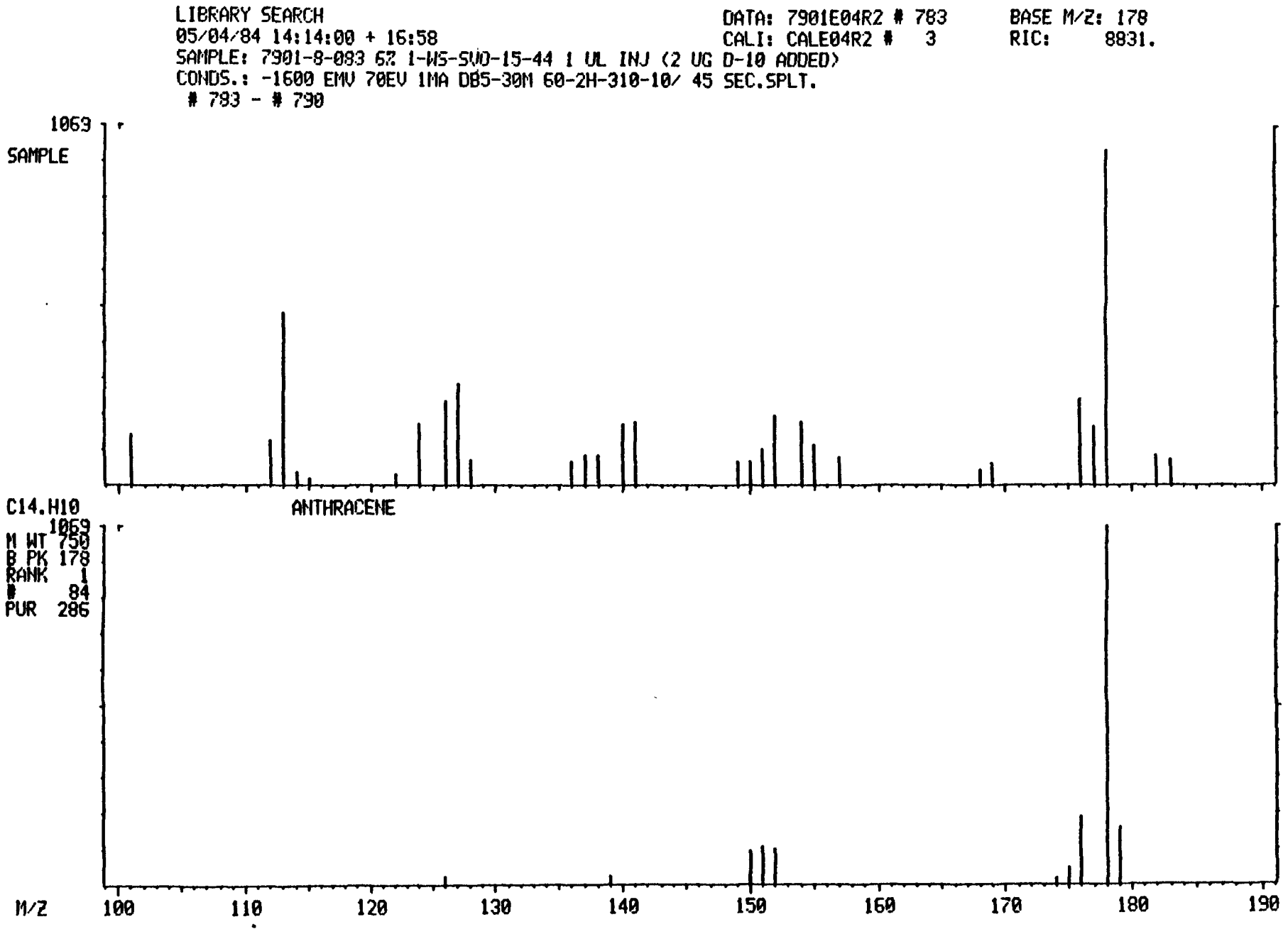


Figure G-14. Mass spectral comparison of anthracene to a peak in NHATS 6% Florisil semivolatile composite.

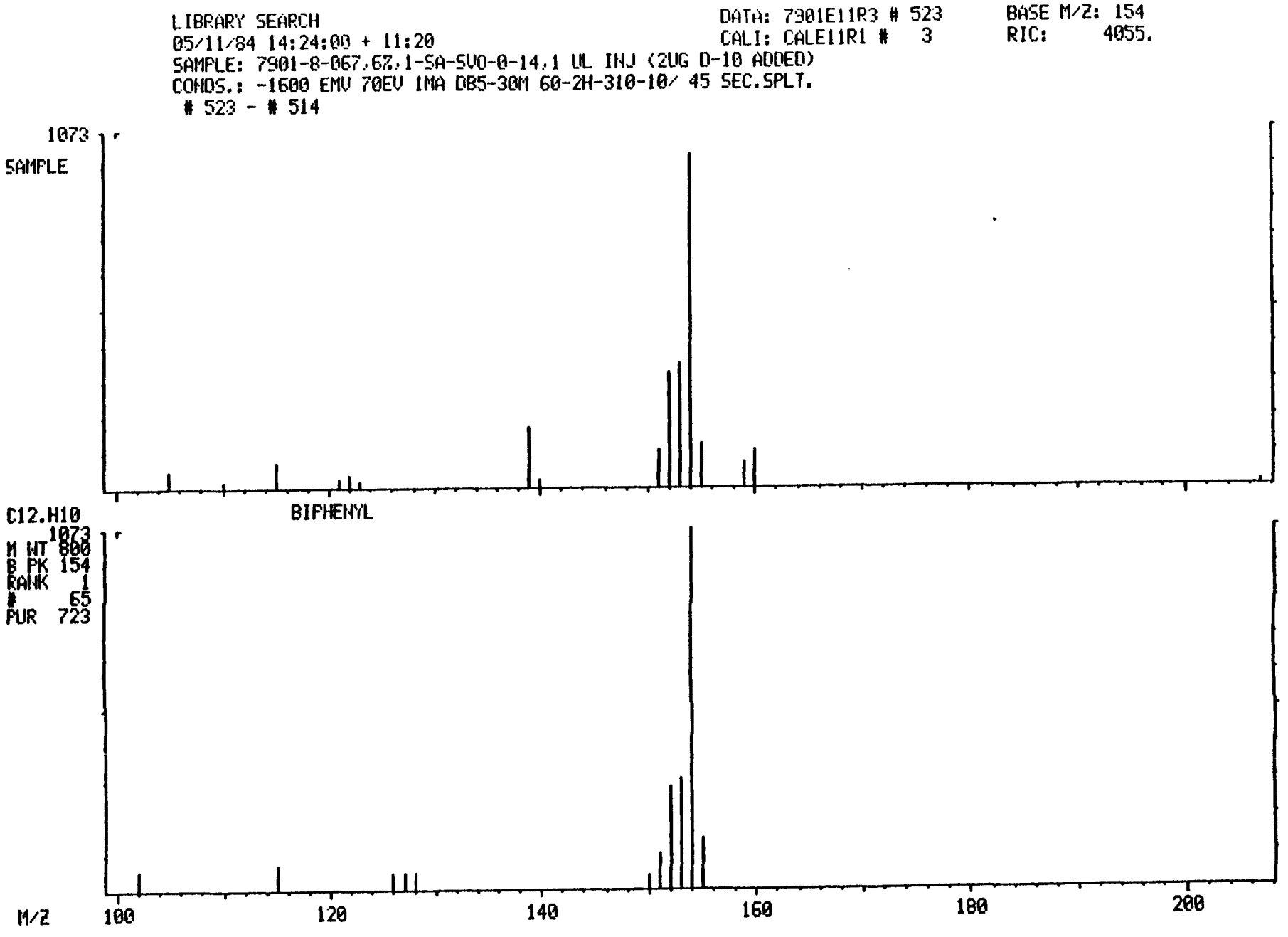


Figure G-15. Mass spectral comparison of biphenyl to a peak in NHATS 6% Florisil semivolatile composite.

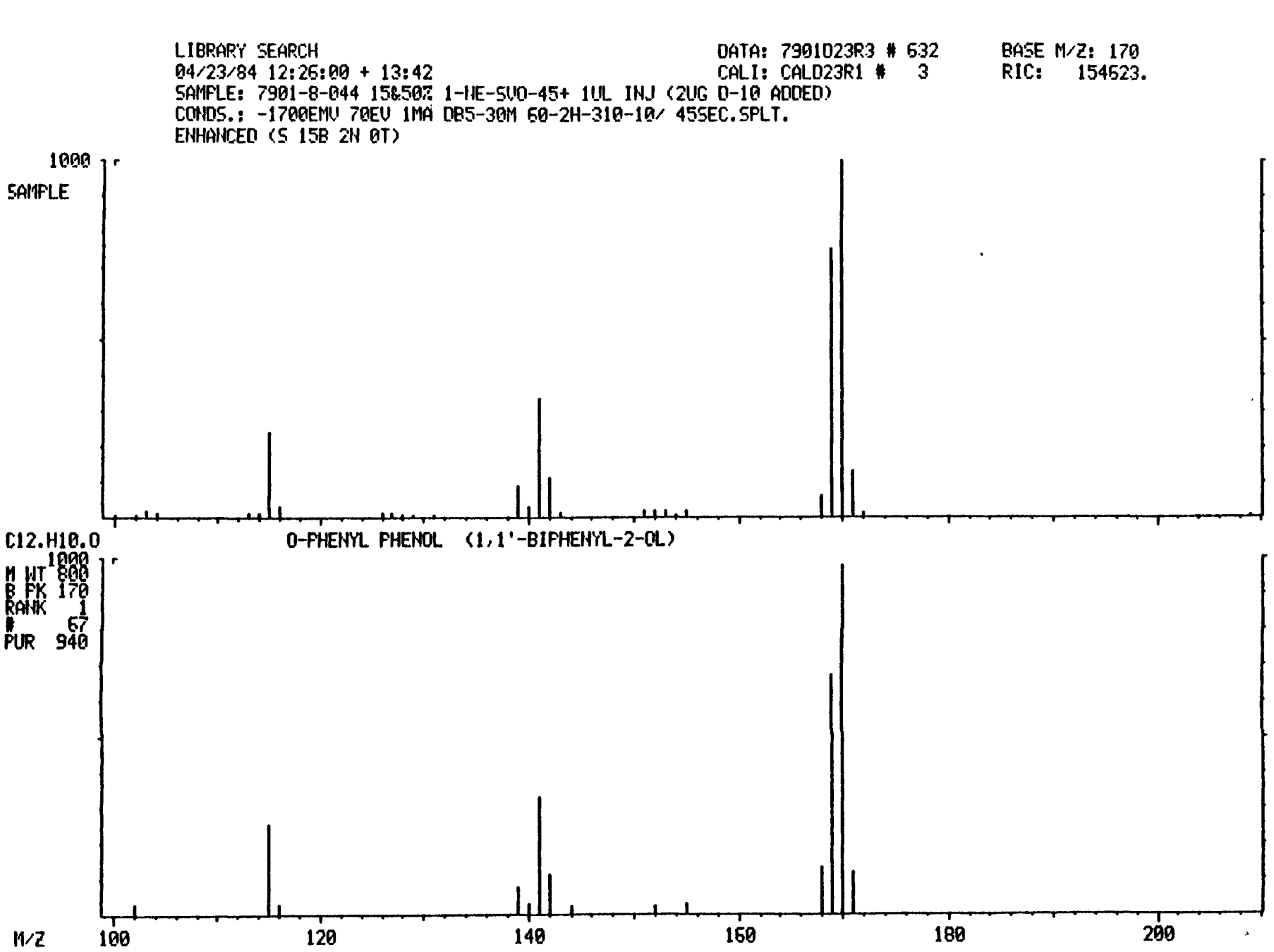


Figure G-32. Mass spectral comparison of o-phenyl phenol to a peak in NHATS 15/50% Florisil semivolatile composite.

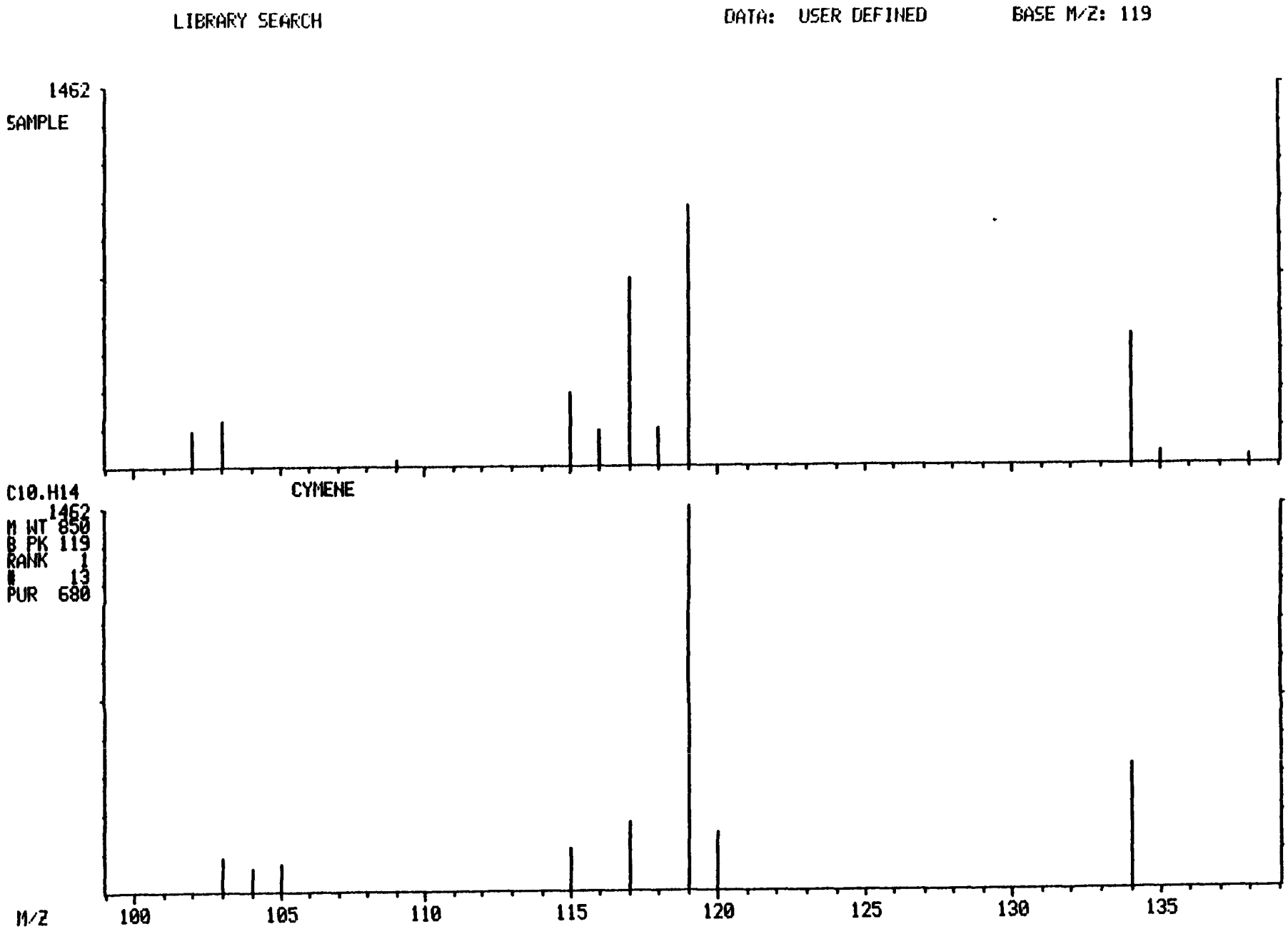


Figure G-17. Mass spectral comparison of cymene to a peak in NHATS 6% Florisil semivolatile composite.

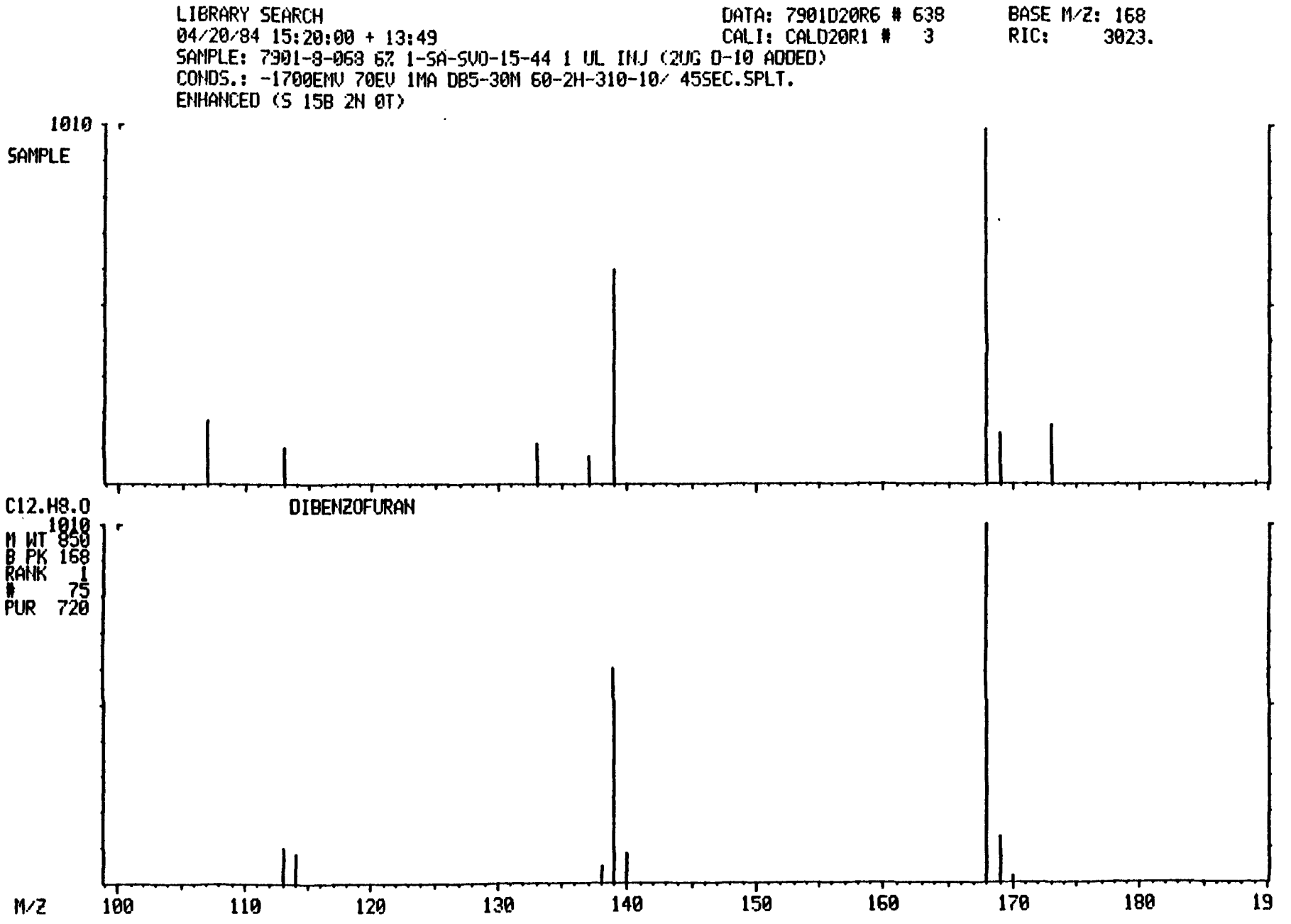
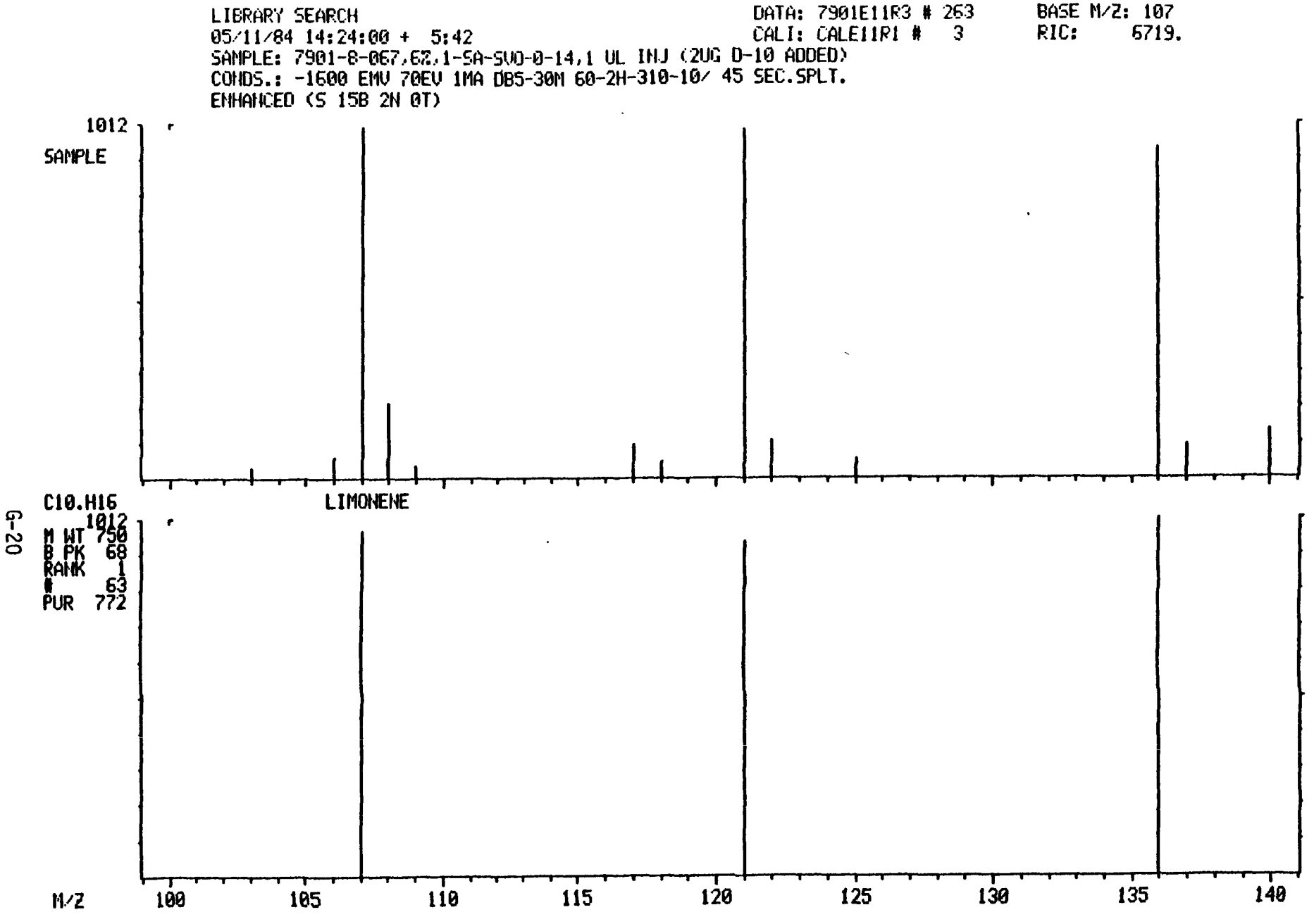


Figure G-18. Mass spectral comparison of dibenzofuran to a peak in NHATS 6% Florisil semivolatile composite.



G-20

Figure G-19. Mass spectral comparison of limonene to a peak in NHATS 6% Florisil semivolatile composite.

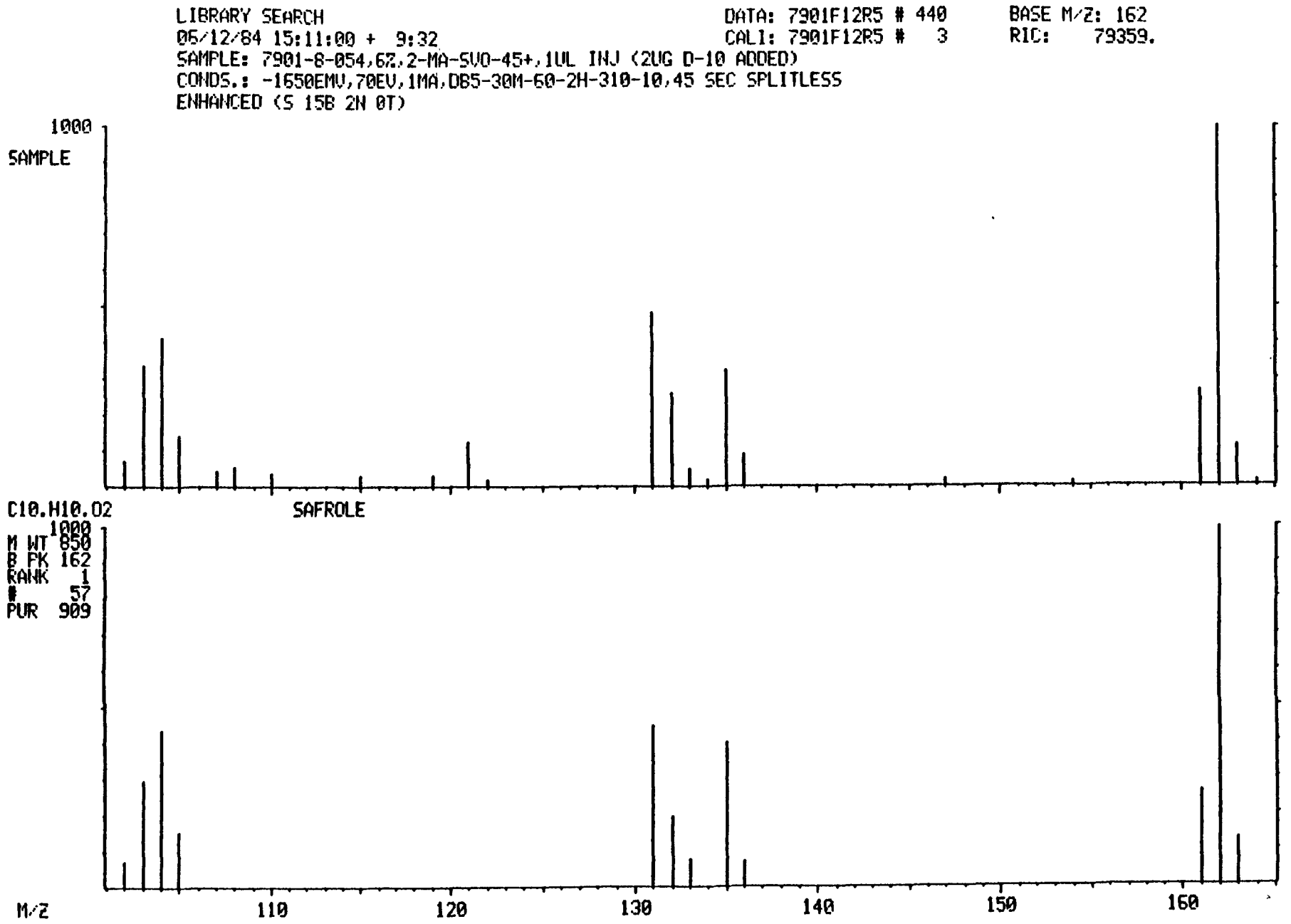


Figure G-20. Mass spectral comparison of safrole to a peak in NHATS 6% Florisil semivolatile composite.

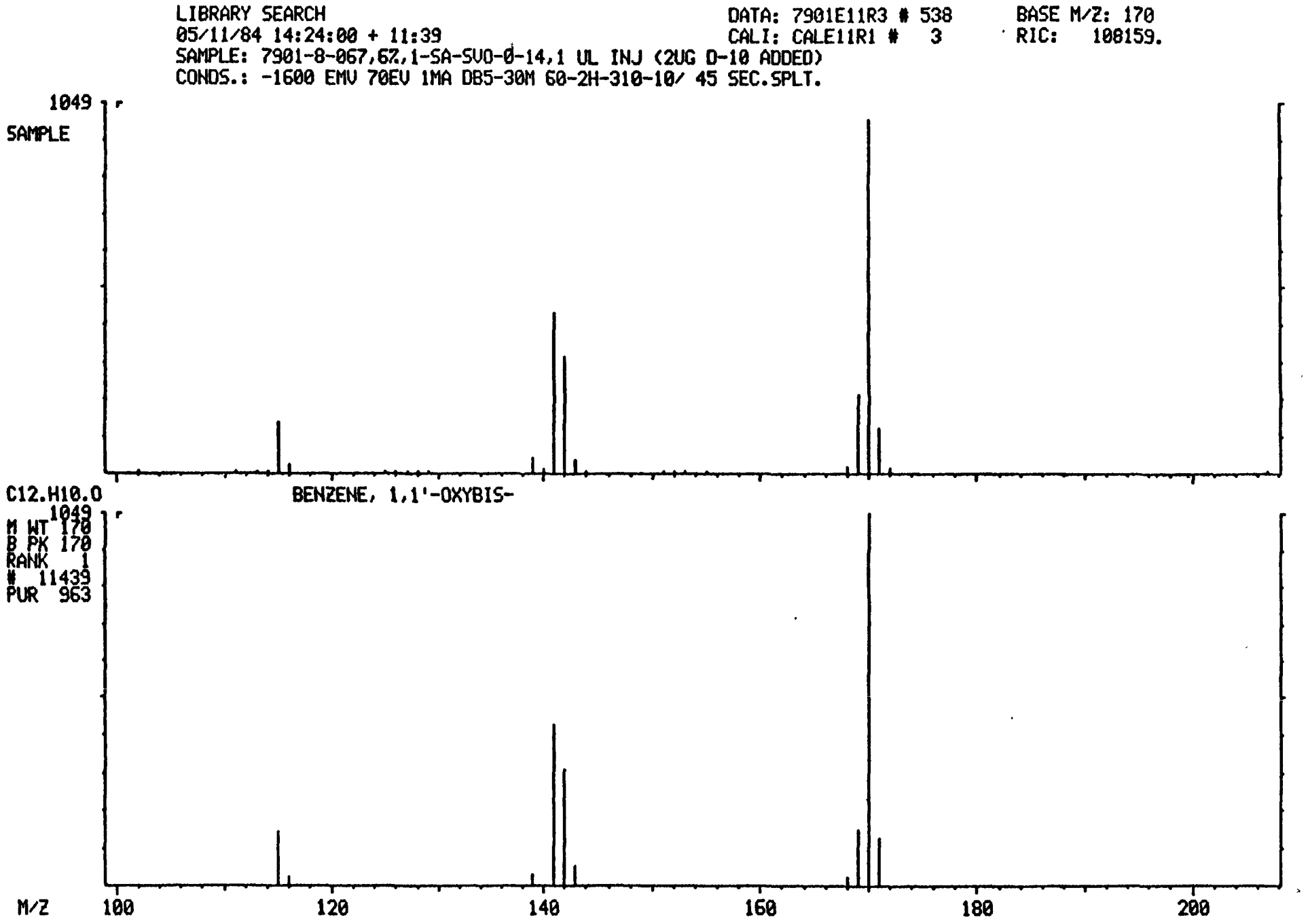


Figure G-21. Mass spectral comparison of diphenyl ether to a peak in NHATS 6% Florisil semivolatile composite.

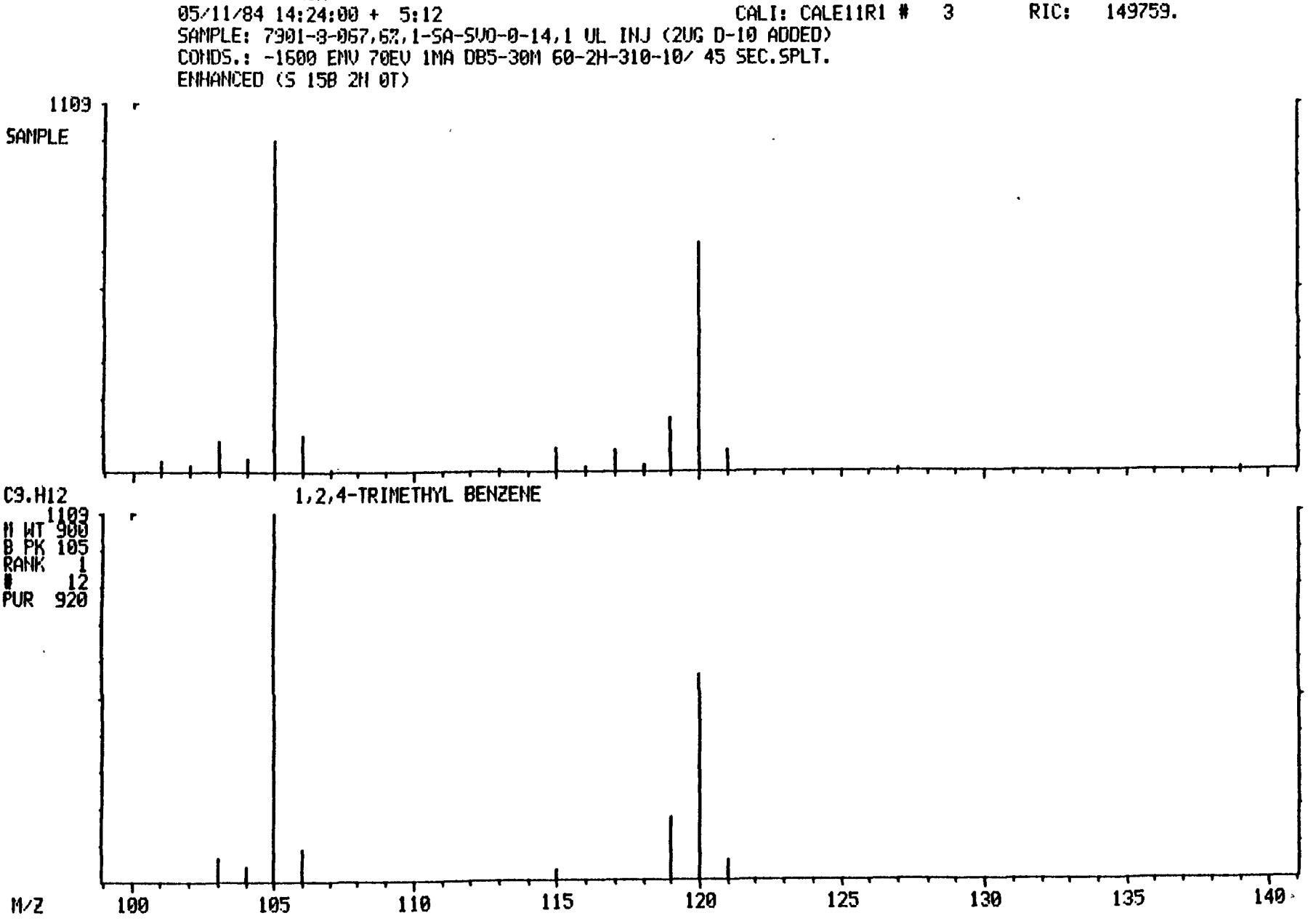


Figure G-22. Mass spectral comparison of 1,2,4-trimethyl benzene to a peak in NHATS 6% Florisil semivolatile composite.

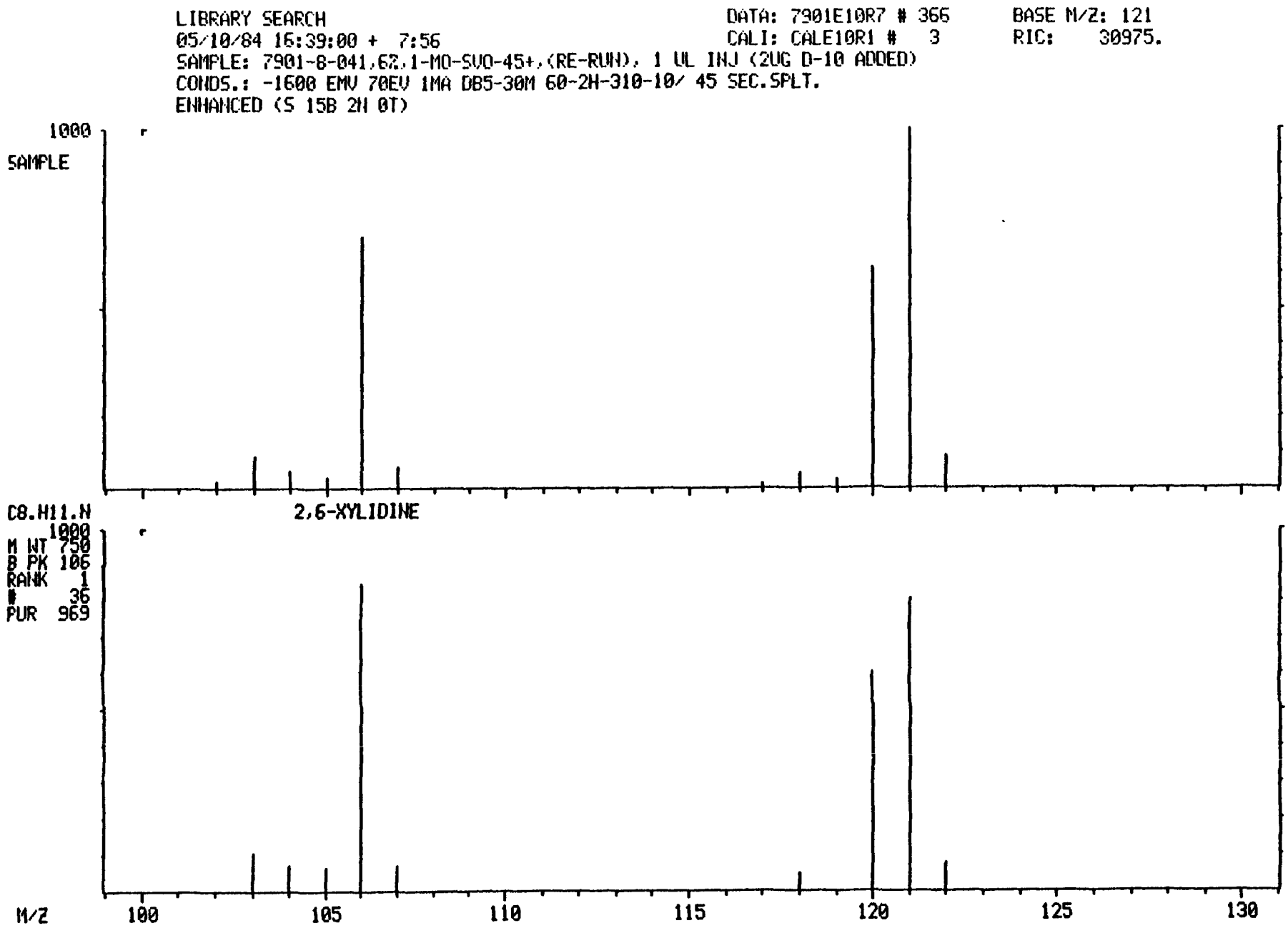


Figure G-23. Mass spectral comparison of 2,6-xylidine to a peak in NHATS 6% Florisil semivolatile composite.

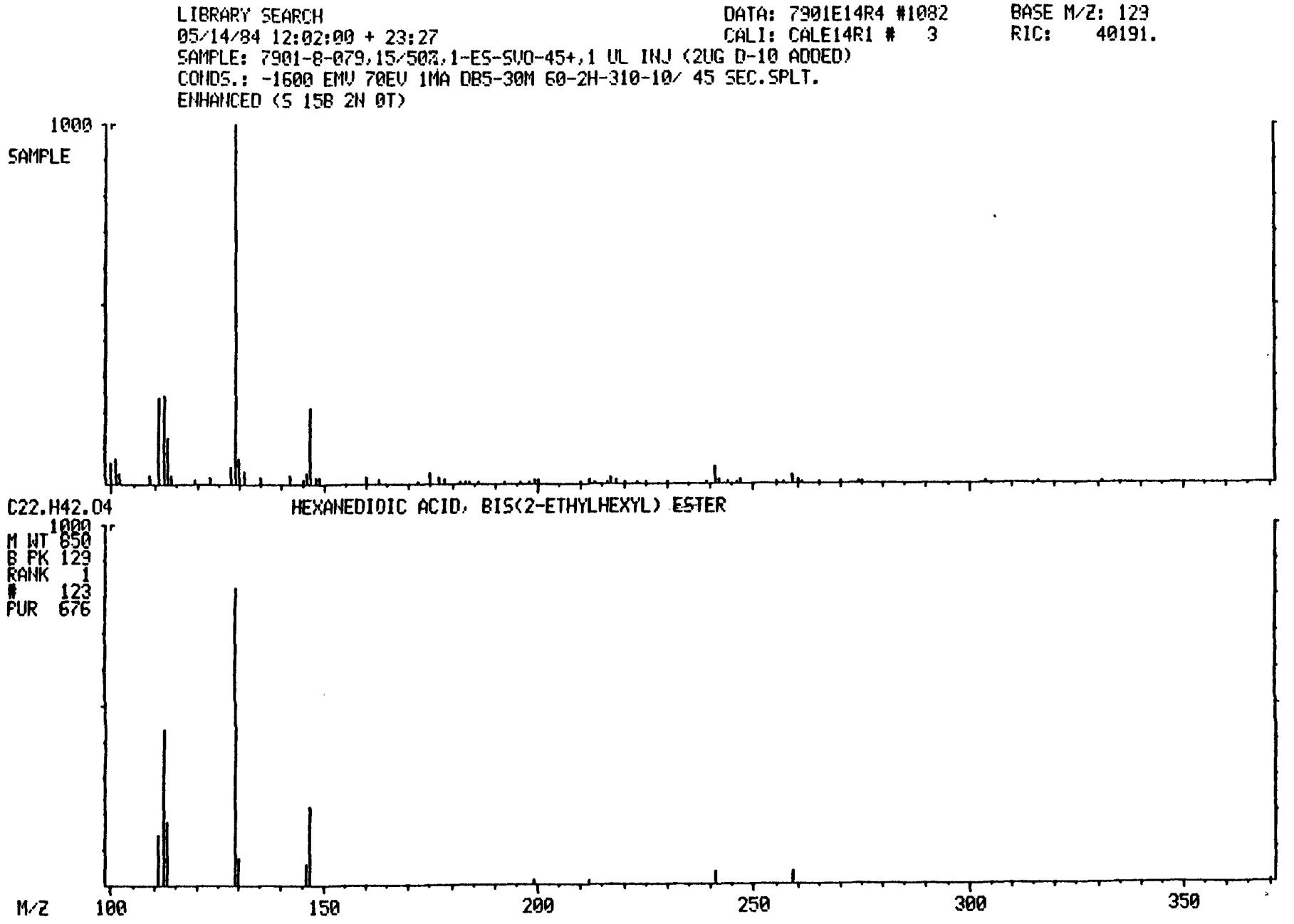


Figure G-24. Mass spectral comparison of bis(2-ethylhexyl) adipate to a peak in NHATS 15/50% Florisil semivolatile composite.

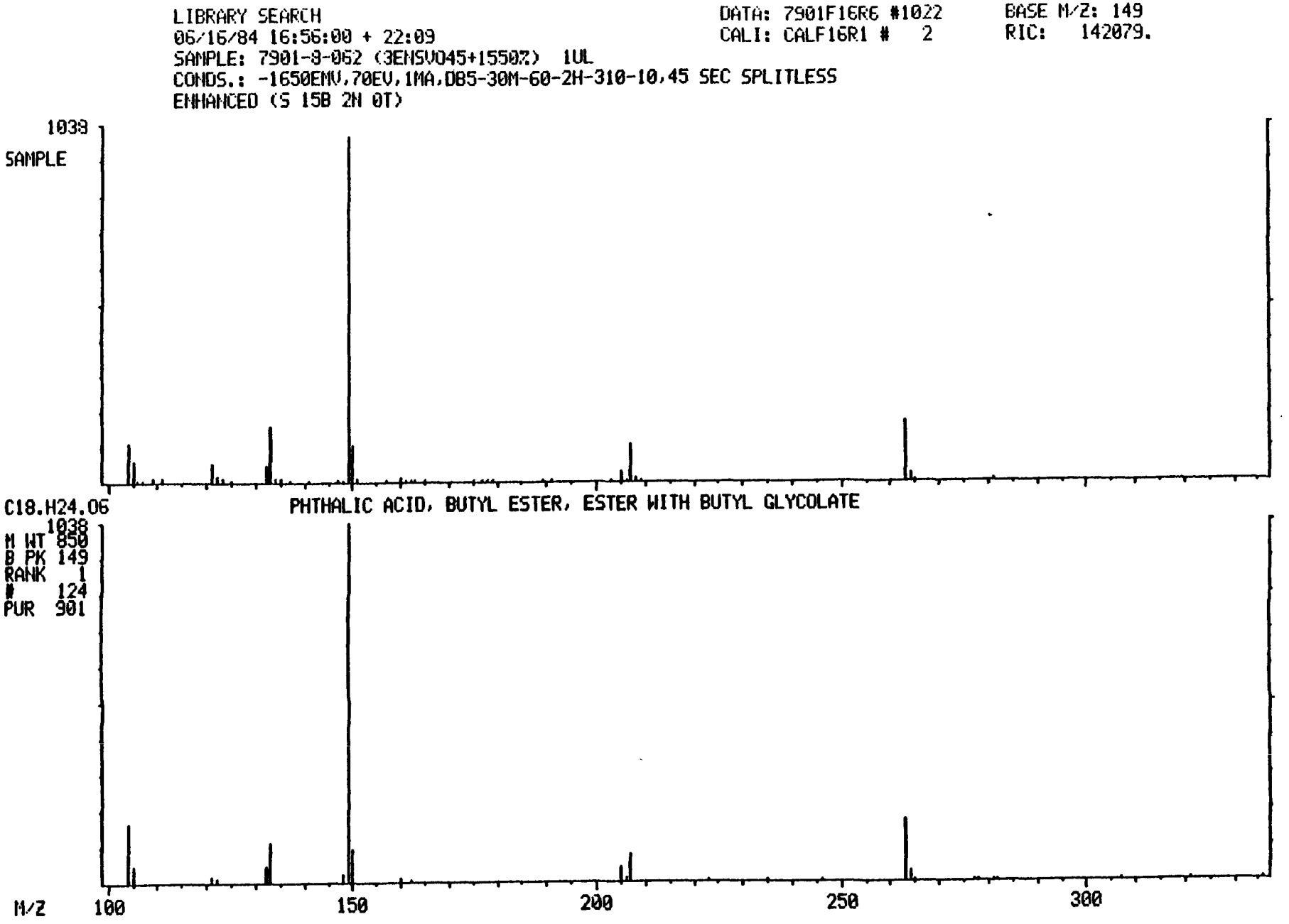


Figure G-25. Mass spectral comparison of butyl phthalate butyl glycolate to a peak in NHATS 15/50% Florisil semivolatile composite.

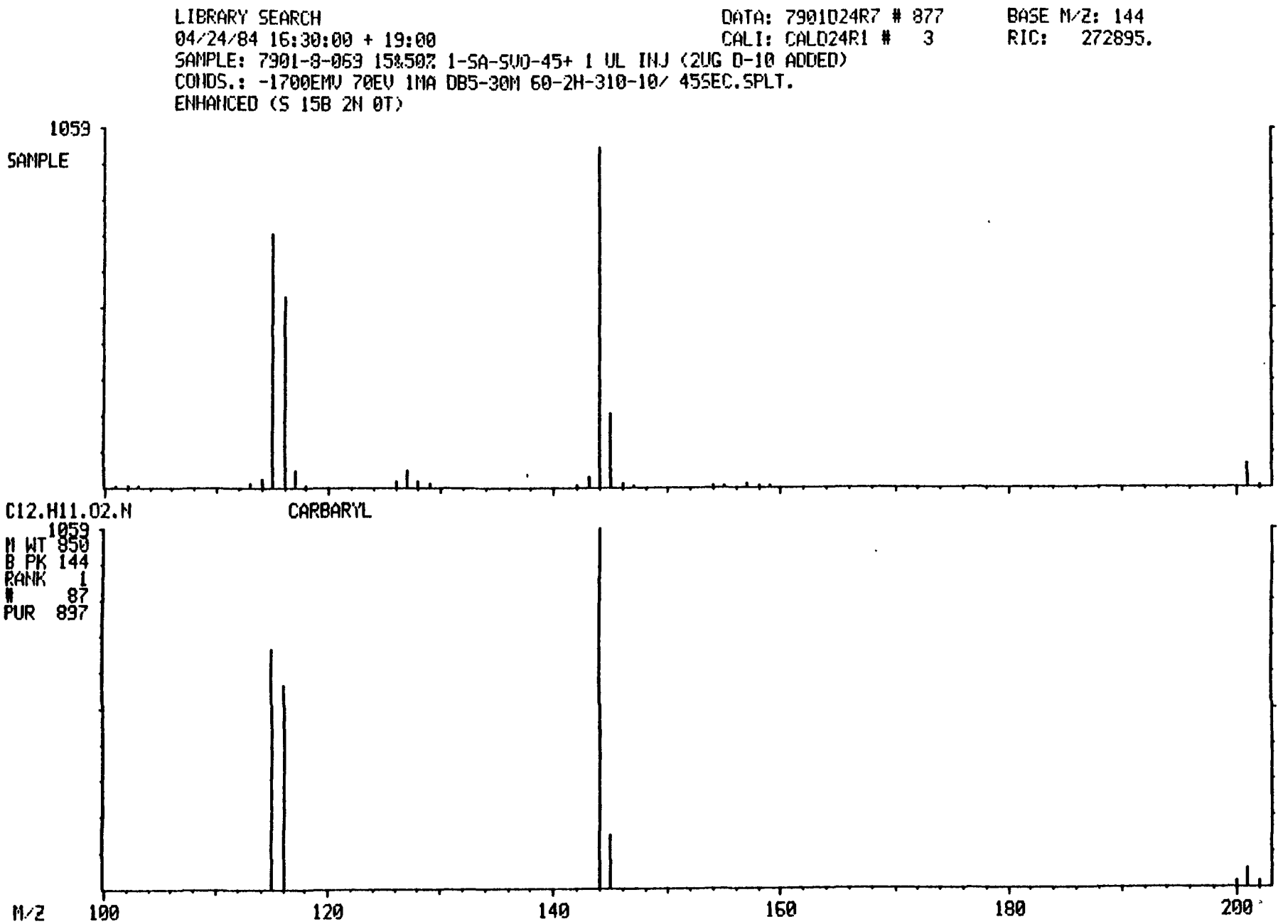


Figure G-26. Mass spectral comparison of carbaryl to a peak in NHATS 15/50% Florisil semivolatile composite.

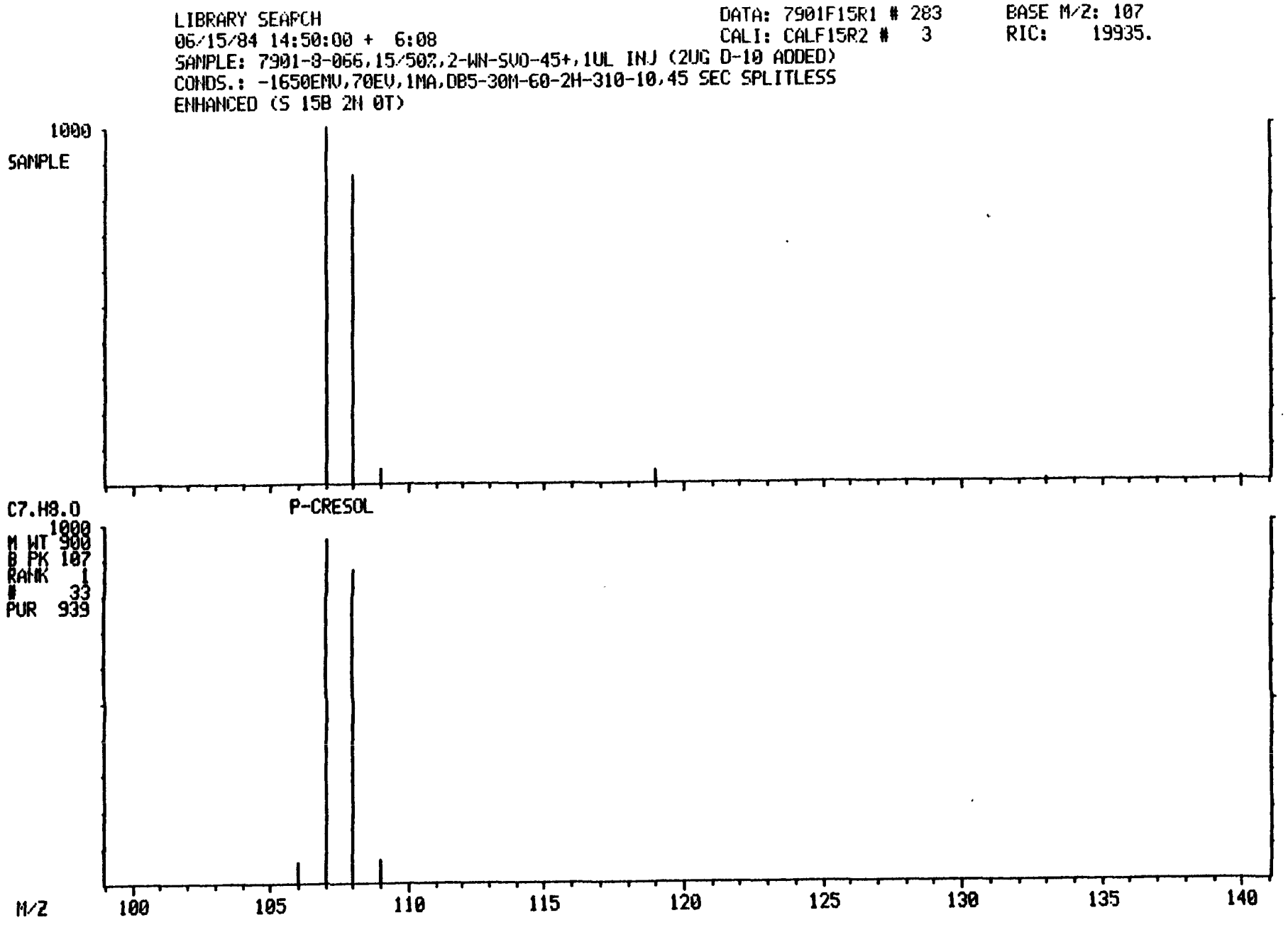


Figure G-27. Mass spectral comparison of p-cresol to a peak in NHATS 15/50% Florisil semivolatile composite.

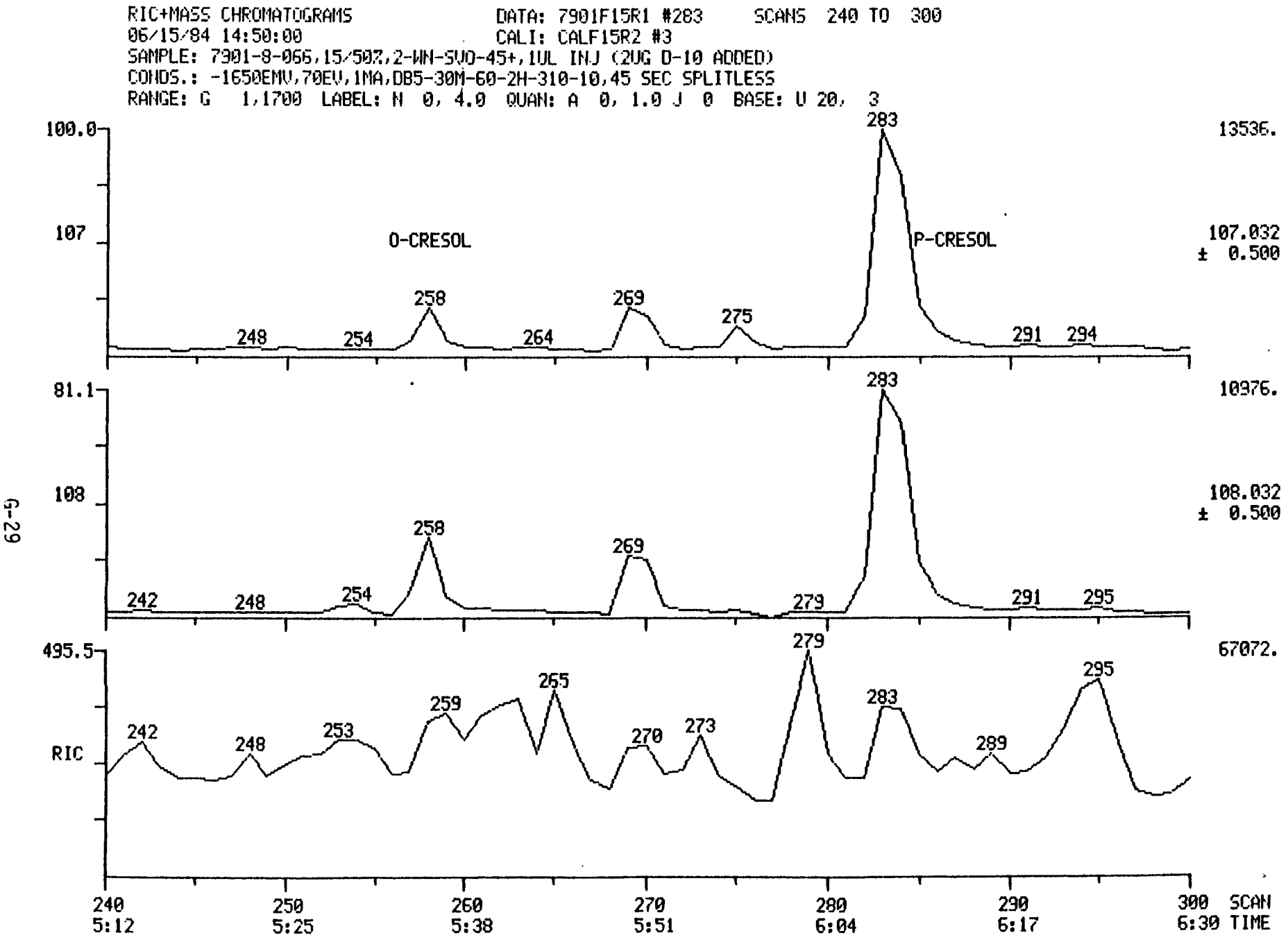


Figure G-28. Mass chromatograms characteristic of cresols, showing distribution of isomers.

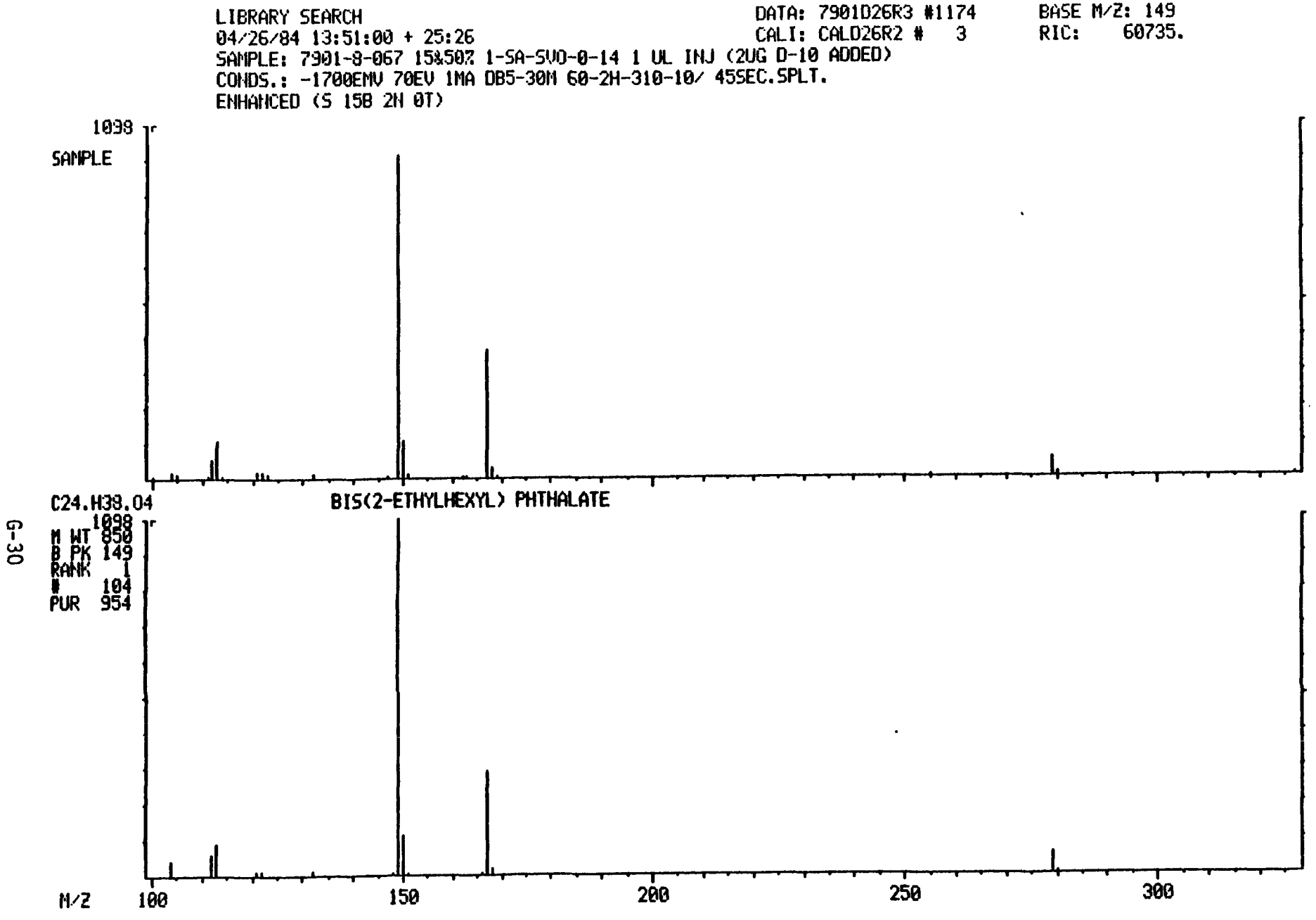


Figure G-29. Mass spectral comparison of bis(2-ethylhexyl) phthalate to a peak in NHATS 15/50% Florisil semivolatile composite.

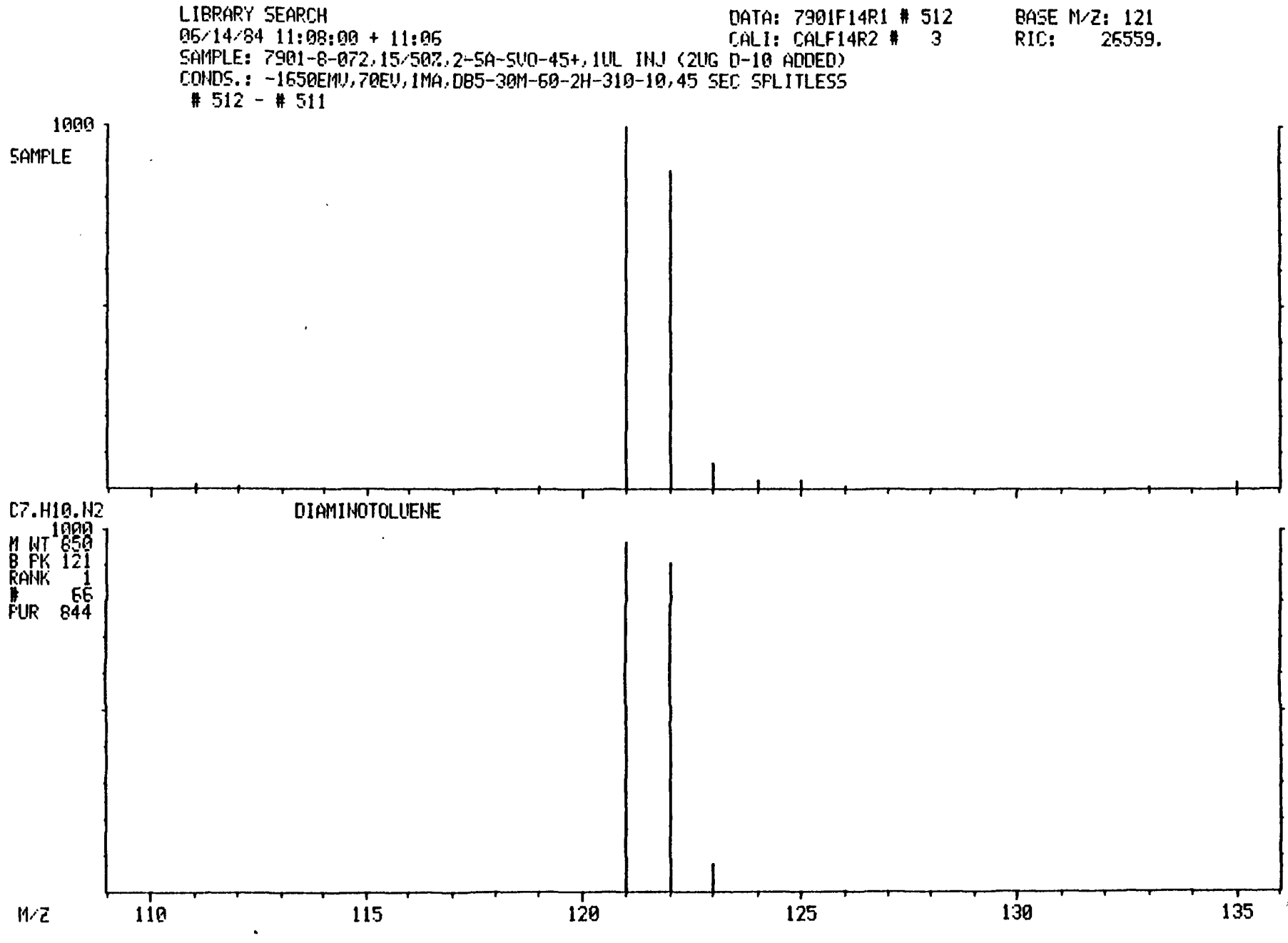


Figure G-30. Mass spectral comparison of diaminotoluene to a peak in NHATS 15/50% Florisil semivolatile composite.

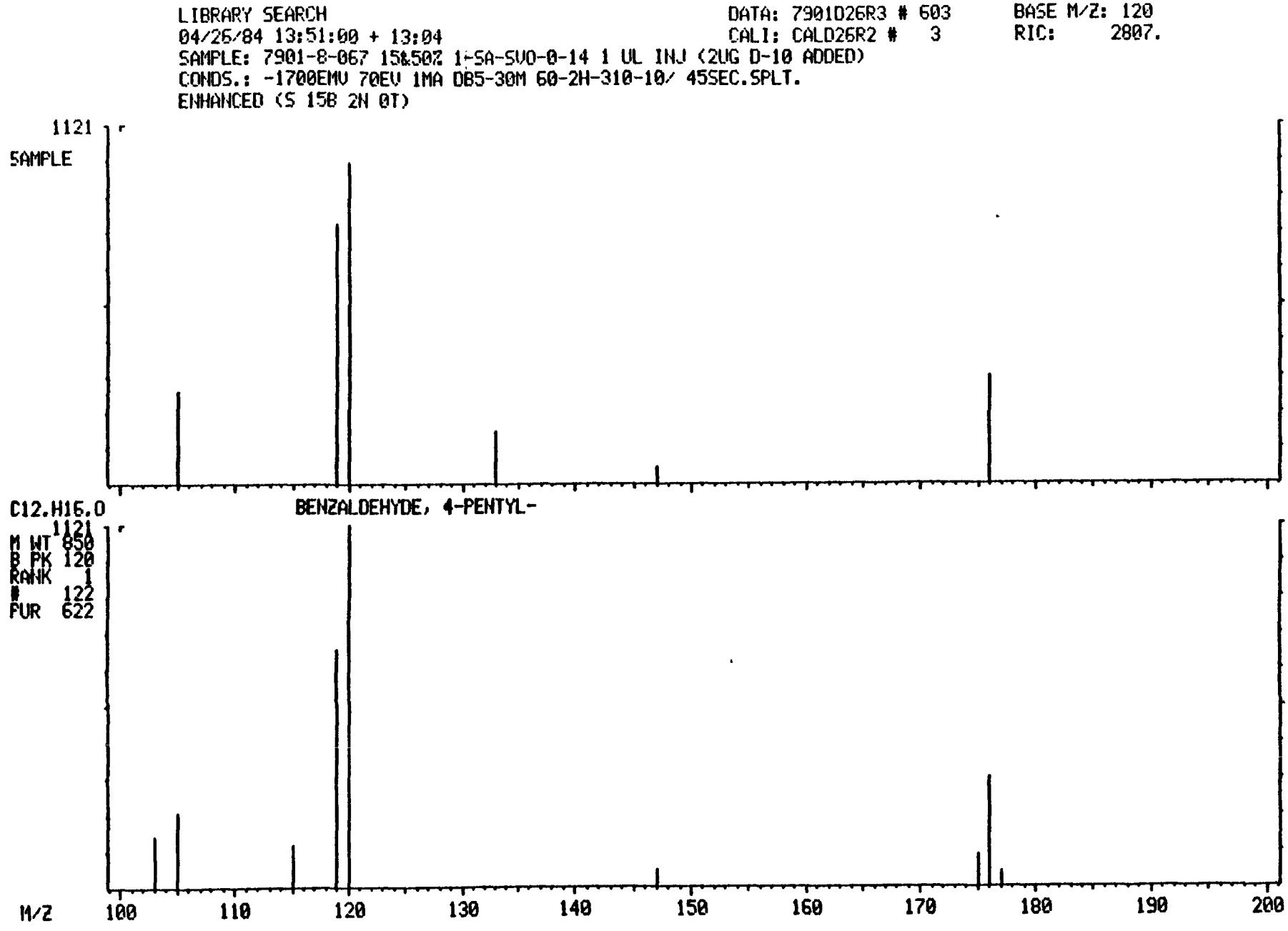


Figure G-31. Mass spectral comparison of 4-pentyl-benzaldehyde to a peak in NHATS 15/50% Florisil semivolatile composite.

50272 - 101

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Jon D. Onstot, John S. Stanley

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425 Volker Boulevard
Kansas City, MO 64110

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15. Supplementary Notes

16. Abstract (Limit: 200 words)

The National Human Adipose Tissue Survey (NHATS), administered by EPA/OTS, is an on-going 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 to determine the occurrence of compounds selected from the Superfund Amendments and Reauthorization Act (SARA) Title III Toxic Chemical Listing, and from the SARA Section 110 CERCLA listing of 100 hazardous substances. A total of 61 volatile and 120 semivolatile target compounds were selected for analysis from these listings based on their predicted suitability to the analytical method.

Application of target compound analysis (TCA) to 46 composited adipose tissue samples resulted in the identification of 13 volatile and 19 semivolatile compounds. Frequency of occurrence data was compiled with respect to three age groups, four census regions and nine census divisions.

17. Document Analysis a. Descriptors
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Chemical Analysis
Gas Chromatography

b. Identifiers/Open-Ended Terms

c. COSATI Field/Group

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