182413

000157

SAMPLE DATA

SW-2

ORGANICS ANALYSIS DATA SHEET

(PAGE 1)

SAMPLE NUMBER

SW-2

Laboratory Name:NANCO LABORATORY INC.
Lab Sample ID No:>P3295
Sample Matrix: WATER
Data Release Authorized By:

Case No: N.J. D.E.P.
QC Report No: 008, 009
Contract No: N/A
Date Sample Received: 9/19/86

VOLATILE COMPOUNDS

000158

Concentration: Low Medium (Circle One)
Date Extracted/Prepared: 09/23/86
Date Analyzed: 09/23/86
Conc/Dil Factor: 1 pH: 7.1
Percent Moisture: N/A

CAS Number		ug/l or ug/Kg (Circle One)	CAS Number		ug/l or ug/Kg (Circle One)
74-87-3	Chloromethane	10.0 U	79-34-5	1,1,2,2-Tetrachloroethane	5.0 U
74-83-9	Bromomethane	10.0 U	78-87-5	1,2-Dichloropropane	5.0 U
75-01-4	Vinyl Chloride	10.0 U	10061-02-6	Trans-1,3-Dichloropropene	5.0 U
75-00-3	Chloroethane	10.0 U	79-01-6	Trichloroethene	5.0 U
75-09-2	Methylene Chloride	3.6 J	124-48-1	Dibromochloromethane	5.0 U
67-64-1	ACETONE	10.0 U	79-00-5	1,1,2-Trichloroethane	5.0 U
75-15-0	Carbon Disulfide	5.0 U	71-43-2	Benzene	5.0 U
75-35-4	1,1-Dichloroethene	5.0 U	10061-01-5	cis-1,3-Dichloropropene	5.0 U
75-34-3	1,1-Dichloroethane	5.0 U	110-75-8	2-Chloroethylvinylether	10.0 U
156-60-5	Trans-1,2-Dichloroethene	5.0 U	75-25-2	Bromoform	5.0 U
67-66-3	Chloroform	5.0 U	591-78-6	2-Hexanone	10.0 U
107-06-2	1,2-Dichloroethane	5.0 U	108-10-1	4-Methyl-2-Pentanone	10.0 U
78-93-3	2-Butanone	10.0 U	127-18-4	Tetrachloroethene	5.0 U
71-55-6	1,1,1-Trichloroethane	5.0 U	108-88-3	Toluene	3.8 JB
56-23-5	Carbon Tetrachloride	5.0 U	108-90-7	Chlorobenzene	5.0 U
108-05-4	Vinyl Acetate	10.0 U	100-41-4	Ethylbenzene	5.0 U
75-27-4	Bromodichloromethane	5.0 U	100-42-5	Styrene	5.0 U
				Total Xylenes	5.0 U

Data Reporting Qualifiers

For reporting results to EPA, the following results qualifiers are used. Additional flags or footnotes explaining results are encouraged. However, the definition of each flag must be explicit.

VALUE

If the result is a value greater than or equal to the detection limit, report the value.

U

Indicates compound was analyzed for but not detected. Report the minimum detection limit for the sample with the U(e.g.10U based on necessary concentration dilution actions. (This is not necessarily the instrument detection limit.) The footnote should read U-Compound was analyzed for but not detected.The number is the minimum attainable detection limit for the sample.

J

Indicates an estimated value.This flag is used either when estimating a concentration for tentatively identified compounds where a 1 1 response is assumed or when the mass spectral data indicates the presence of a compound that meets the identification criteria but the result is less than the specified detection limit but greater than zero (e.g. 10J).

C

This flag applies to pesticide parameters where the identification has been confirmed by GC/MS Single component pesticides greater than or equal to 10 ng/ul in the final extract should be confirmed by GC/MS

B

This flag is used when the analyte is found in the blank as well as a sample. It indicates possible/probable blank contamination and warns the data user to take appropriate action.

OTHER

Other specific flags and footnotes may be required to properly define the results. If used, they must be fully described and such description attached to the data summary report.

ORGANIC ANALYSIS DATA SHEET
(PAGE 2)

000159

LABORATORY NAME: NANCO LABS. INC.
CASE NO: N.J.D.E.P.

SAMPLE NO.
SW-2

SEMIVOLATILE COMPOUNDS

Concentration: Low Medium (Circle One)
Date Extracted/Prepared: 9/23/86
Date Analyzed: 10/22/86
Conc/Dil Factor:----------> 1
Percent Moisture: N/A

GPC Cleanup: Yes____ No X
Separatory Funnel Extraction: Yes X
Continuous Liquid - Liquid Extraction: Yes___

CAS Number		ug/l or ug/Kg (Circle One)
62-75-9	N-Nitrosodimethylamine	10.0 U
108-95-2	Phenol	10.0 U
62-53-3	Aniline	10.0 U
111-44-4	bis(-2-Chloroethyl)Ether	10.0 U
95-57-8	2-Chlorophenol	10.0 U
541-73-1	1,3-Dichlorobenzene	10.0 U
106-46-7	1,4-Dichlorobenzene	10.0 U
100-51-6	Benzyl Alcohol	10.0 U
95-50-1	1,2-Dichlorobenzene	10.0 U
95-48-7	2-Methylphenol	10.0 U
39638-32-9	bis(2-chloroisopropyl)Ether	10.0 U
106-44-5	4-Methylphenol	10.0 U
621-64-7	N-Nitroso-Di-n-Propylamine	10.0 U
67-72-1	Hexachloroethane	10.0 U
98-95-3	Nitrobenzene	10.0 U
78-59-1	Isophorone	10.0 U
88-75-5	2-Nitrophenol	10.0 U
105-67-9	2,4-Dimethylphenol	10.0 U
65-85-0	Benzoic Acid	50.0 U
111-91-1	bis(-2-Chloroethoxy)Methane	10.0 U
120-83-2	2,4-Dichlorophenol	10.0 U
120-82-1	1,2,4-Trichlorobenzene	10.0 U
91-20-3	Naphthalene	3.3 J
106-47-8	4-Chloroaniline	15.0
87-68-3	Hexachlorobutadiene	10.0 U
59-50-7	4-Chloro-3-Methylphenol	10.0 U
91-57-6	2-Methylnaphthalene	24.0
77-47-4	Hexachlorocyclopentadiene	10.0 U
88-06-2	2,4,6-Trichlorophenol	10.0 U
95-95-4	2,4,5-Trichlorophenol	50.0 U
91-58-7	2-Chloronaphthalene	10.0 U
88-74-4	2-Nitroaniline	50.0 U
131-11-3	Dimethyl Phthalate	10.0 U
208-96-8	Acenaphthylene	10.0 U
99-09-2	3-Nitroaniline	50.0 U

CAS Number		ug/l or ug/Kg (Circle One)
83-32-9	Acenaphthene	10.0 U
51-28-5	2,4-Dinitrophenol	50.0 U
100-02-7	4-Nitrophenol	50.0 U
132-64-9	Dibenzofuran	10.0 U
121-14-2	2,4-Dinitrotoluene	13.0
606-20-2	2,6-Dinitrotoluene	10.0 U
84-66-2	Diethylphthalate	10.0 U
7005-72-3	4-Chlorophenyl-phenylether	10.0 U
86-73-7	Fluorene	10.0
100-01-6	4-Nitroaniline	50.0 U
534-52-1	4,6-Dinitro-2-Methylphenol	50.0 U
86-30-6	N-Nitrosodiphenylamine (1)	53.0
101-55-3	4-Bromophenyl-phenylether	10.0 U
118-74-1	Hexachlorobenzene	10.0 U
87-86-5	Pentachlorophenol	50.0 U
85-01-8	Phenanthrene	19.0
120-12-7	Anthracene	10.0 U
84-74-2	Di-n-Butylphthalate	10.0 U
206-44-0	Fluoranthene	10.0 U
92-87-5	Benzidine	80.0 U
129-00-0	Pyrene	10.0 U
85-68-7	Butylbenzylphthalate	10.0 U
91-94-1	3,3'-Dichlorobenzidine	20.0 U
56-55-3	Benzo(a)Anthracene	10.0 U
117-81-7	bis(2-Ethylhexyl)Phthalate	77.0 B
218-01-9	Chrysene	10.0 U
117-84-0	Di-n-Octyl Phthalate	65.0
205-99-2	Benzo(b)Fluoranthene	10.0 U
207-08-9	Benzo(k)Fluoranthene	10.0 U
50-32-8	Benzo(a)Pyrene	10.0 U
193-39-5	Indeno(1,2,3-cd)Pyrene	10.0 U
53-70-3	Dibenz(a,h)Anthracene	10.0 U
191-24-2	Benzo(g,h,i)Perylene	10.0 U

(1) - Cannot be separated from diphenylamine

ORGANICS ANALYSIS DATA SHEET
(PAGE 3)

000160 SAMPLE NUMBER

SW 2

LABORATORY NAME: NANCO LABS, INC.
CASE NO: NJ DEP

PESTICIDE/PCBs

Concentration: Low Medium (Circle One)
Date Extracted/Prepared: 9/23/86
Date Analyzed: 10/2/86
Conc/Dil Factor: -----> 1
Percent Moisture: N/A

GPC Cleanup: Yes___ No_X_
Separatory Funnel Extraction: Yes_X_
Continuous Liquid-Liquid Extraction: Yes___

CAS Number		ug/l or ug/Kg (Circle One)
319-84-6	Alpha-BHC	0.05 U
319-85-7	Beta-BHC	0.05 U
319-86-8	Delta-BHC	0.05 U
58-89-9	Gamma-BHC (Lindane)	0.05 U
76-44-8	Heptachlor	0.05 U
309-00-2	Aldrin	0.05 U
1024-57-3	Heptachlor Epoxide	0.05 U
959-98-8	Endosulfan I	0.05 U
60-57-1	Dieldrin	0.10 U
72-55-9	4,4'-DDE	0.10 U
72-20-8	Endrin	0.10 U
33213-65-9	Endosulfan II	0.10 U
72-54-8	4,4'-DDD	0.10 U
7421-93-4	Endrin Aldehyde	0.10 U
1031-07-8	Endosulfan Sulfate	0.10 U
50-29-3	4,4'-DDT	0.10 U
53494-70-5	Endrin Ketone	0.10 U
72-43-5	Methoxychlor	0.50 U
57-74-9	Chlordane	0.50 U
8001-35-2	Toxaphene	1.00 U
12674-11-2	Aroclor-1016	0.50 U
11104-28-2	Aroclor-1221	0.50 U
11141-16-5	Aroclor-1232	0.50 U
53469-21-9	Aroclor-1242	0.50 U
12672-29-6	Aroclor-1248	0.50 U
11097-69-1	Aroclor-1254	1.00 U
11096-82-5	Aroclor-1260	1.00 U

Vi = Volume of extract injected (ul)

Vs = Volume of water extracted (ml)

Ws = Weight of sample extracted (g)

Vt = Volume of total extract (ul)

Vs 1000 or Ws _____ Vt 10000 Vi 3

FORM I

ORGANICS ANALYSIS DATA SHEET
(PAGE 4)

SAMPLE NUMBER

SW-2

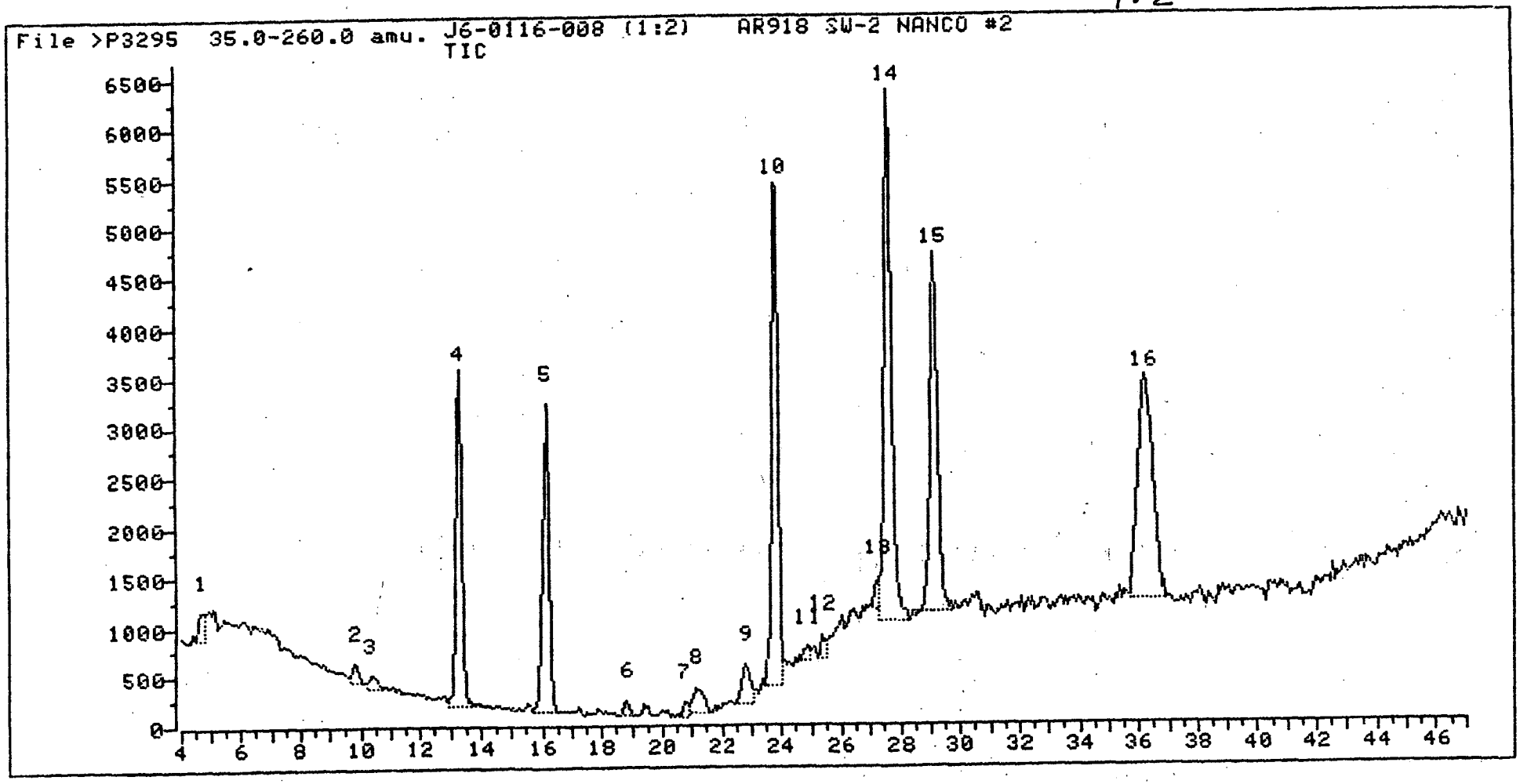
LABORATORY NAME :NANCO LABS.INC.
CASE NO: N.J. D.E.P.

Tentatively Identified Compounds

	CAS Number	Compound Name	Fraction	RT or Scan Number	Estimated Concentration (ug/l or ug/Kg)
1	19812498	2-METHYL AZETIDINE	VOA	22.83	5.1 J
2					
3	-----	UNKNOWN HYDROCARBON	BNA	17.04	310.0 J
4	-----	UNKNOWN HYDROCARBON	BNA	17.32	120.0 J
5	-----	UNKNOWN POLYAROMATIC HYDROCARBON	BNA	18.99	56.0 J
6	-----	UNKNOWN HYDROCARBON	BNA	20.37	130.0 J
7	629594	TETRADECANE	BNA	20.80	920.0 J
8	-----	ISOMER OF DIMETHYL NAPTHALENE	BNA	21.25	130.0 J
9	-----	UNKNOWN HYDROCARBON	BNA	21.60	280.0 J
10	-----	UNKNOWN HYDROCARBON	BNA	21.84	330.0 J
11	-----	UNKNOWN HYDROCARBON	BNA	22.48	740.0 J
12	-----	ISOMER OF NAPHTHALENE	BNA	23.33	140.0 J
13	544763	HEXADECANE	BNA	24.04	950.0 J
14	-----	UNKNOWN	BNA	24.89	200.0 J
15	629787	HEPTADECANE	BNA	25.51	800.0 J
16	1921706	PENTADECANE,2,6,10,14-TETRAMETHYL	BNA	25.60	450.0 J
17	-----	UNKNOWN HYDRCARBON	BNA	26.11	150.0 J
18	638368	HEXADECANE	BNA	27.03	320.0 J
19	-----	UNKNOWN HYDRCARBON	BNA	27.44	96.0 J
20	-----	UNKNOWN HYDRCARBON	BNA	28.22	580.0 J
21	-----	UNKNOWN HYDRCARBON	BNA	29.46	440.0 J
22	-----	UNKNOWN HYDRCARBON	BNA	29.93	110.0 J
23	-----	UNKNOWN HYDRCARBON	BNA	30.67	290.0 J
24	-----	UNKNOWN HYDRCARBON	BNA	31.12	110.0 J
25	-----	UNKNOWN HYDRCARBON	BNA	31.82	240.0 J
26	-----	UNKNOWN HYDRCARBON	BNA	32.92	130.0 J

Inj 9/23/86 9:46

1:2



PK#		
4	BROMOCHLOROMETHANE	(IS)
10	1,4-DIFLUOROBENZENE	(IS)
15	CHLOROBENZENE-d5	(IS)
5	1,2-DICHLOROETHANE-d4	(SR)
14	TOLUENE-d8	(SR)
16	4-BROMOFLUOROBENZENE	(SR)

000162

QUANT REPORT

Operator ID: DALY
Output File: ^P3295::PS
Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2

Quant Rev: 4
Quant Time: 860923 10:35
Injected at: 860923 09:46
Dilution Factor: 2.00

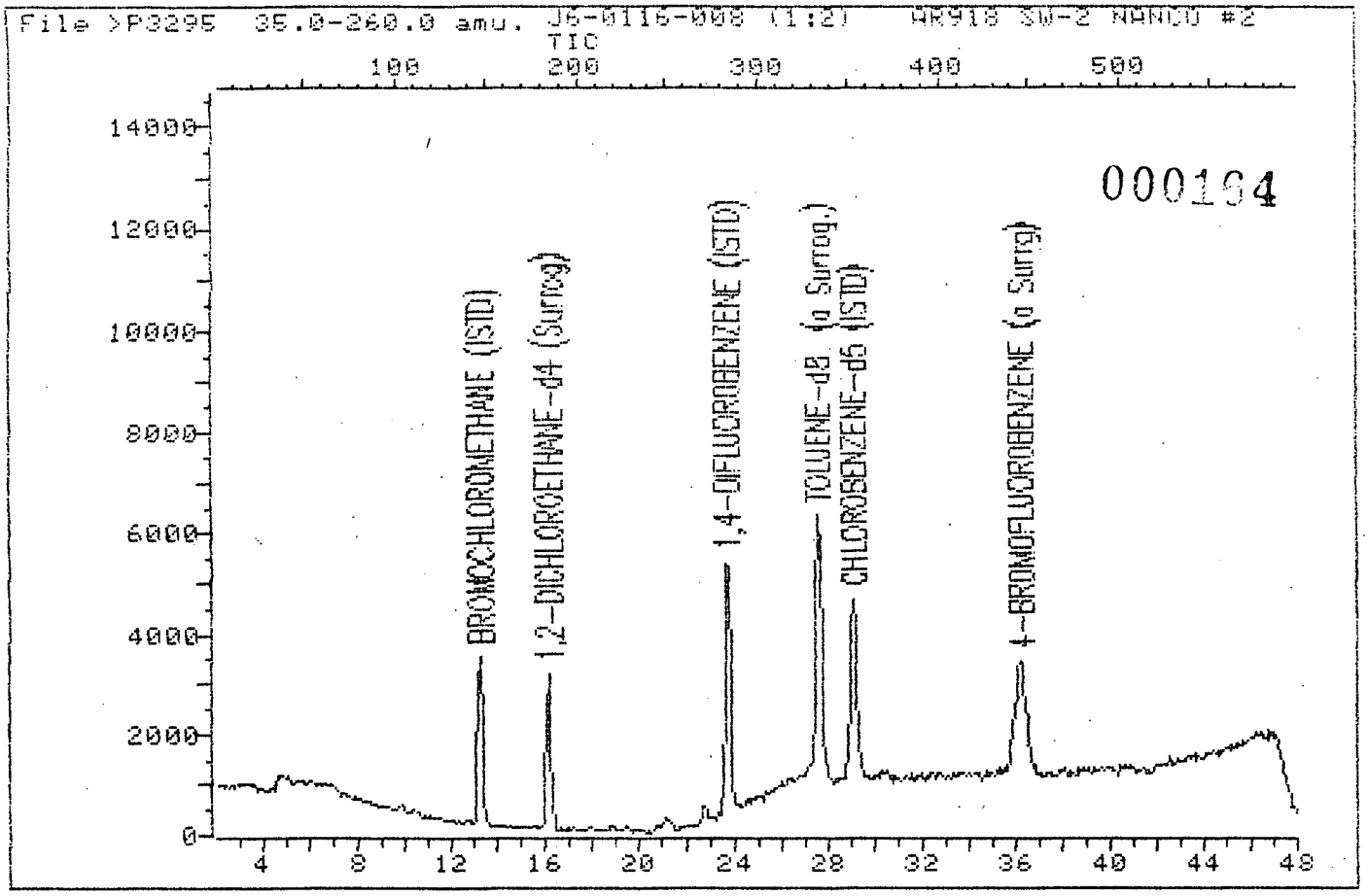
000163

ID File: IDEPA2::NA
Title: IDEPA VOA
Last Calibration: 860923 07:47

	Compound	R.T.	Scan#	Area	Conc	Units	q
1)	*BROMOCHLOROMETHANE (ISTD)	13.30	147	5809	50.00	UG	68
6)	Methylene Chloride	9.84	102	516	3.59	UG	87
14)	*1,4-DIFLUOROBENZENE (ISTD)	23.76	283	26282	50.00	UG	96
29)	*CHLOROBENZENE-d5 (ISTD)	29.14	353	18952	50.00	UG	94
34)	Toluene	27.83	336	881	3.82	UG	82
39)	TOLUENE-d8 (a Surrog.)	27.60	333	25794	98.84	UG	97
40)	4-BROMOFLUOROBENZENE (a Surrg)	36.22	445	18154	107.72	UG	87
41)	*[BROMOCHLOROMETHANE (ISTD)]	13.30	147	5809	50.00	UG	68
42)	1,2-DICHLOROETHANE-d4 (Surrog)	16.14	184	14038	94.48	UG	96

* Compound is ISTD

TOTAL ION CHROMATOGRAM



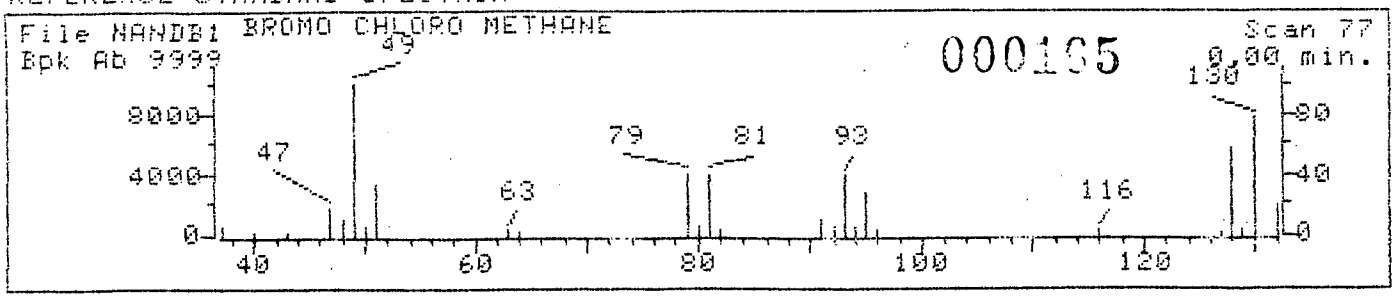
000194

Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2

Id File: IDEPA2::NA
Title: IDEPA VOA
Last Calibration: 860923 07:47

Operator ID: DALY
Quant Time: 860923 10:35
Injected at: 860923 09:46

REFERENCE STANDARD SPECTRUM



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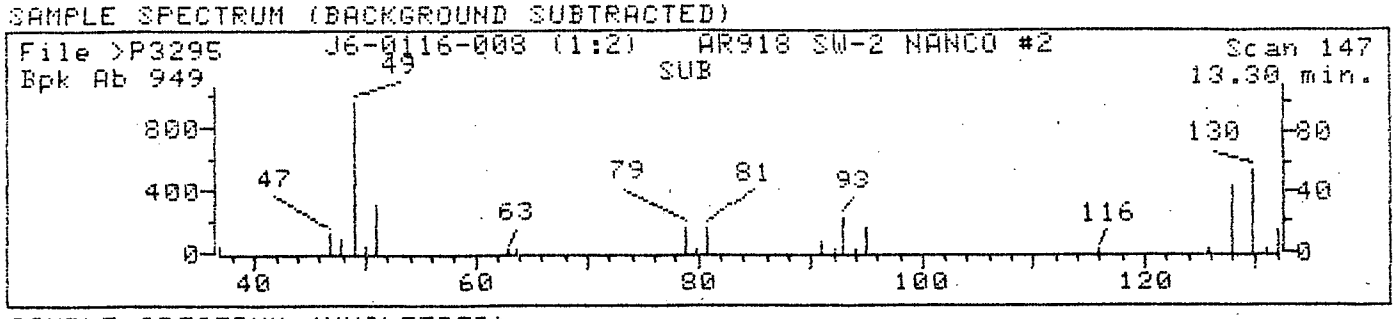

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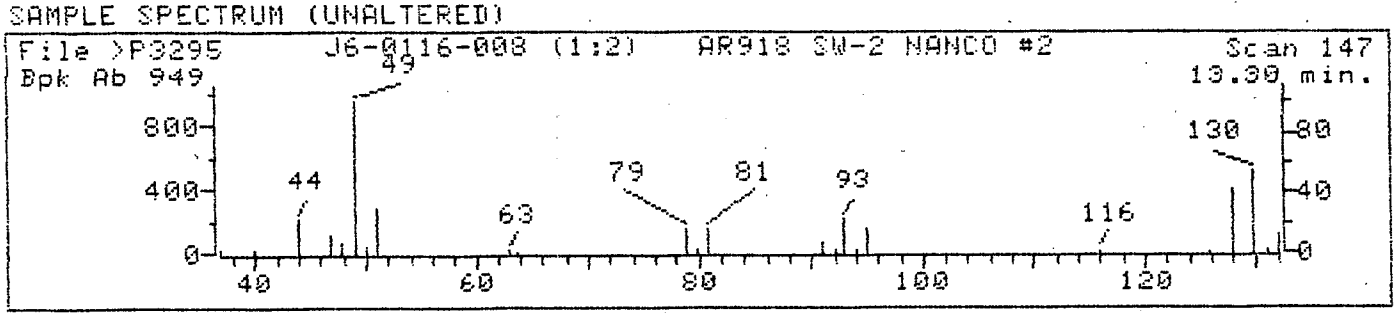
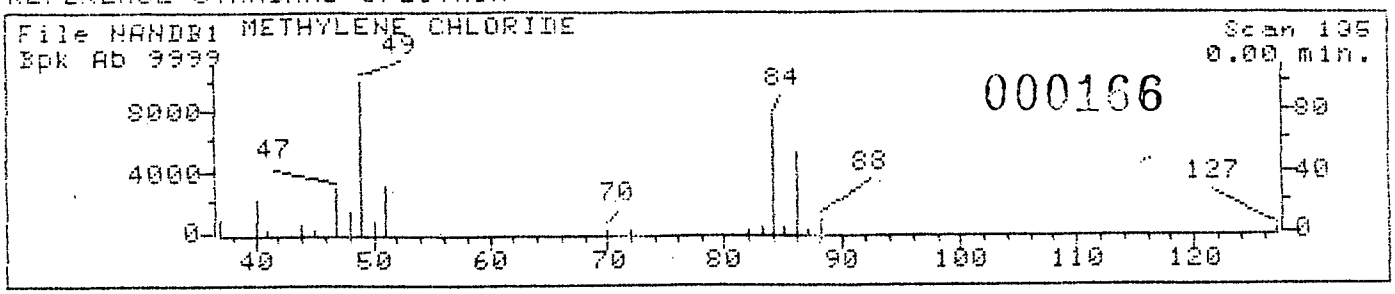


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

Compound No: 1 (ISTD)
Compound Name: BROMOCHLOROMETHANE (ISTD)
Scan Number: 147
Retention Time: 13.30 min.
Area: 5809
Concentration: 50.00 UG
a-value: 68

plg

REFERENCE STANDARD SPECTRUM



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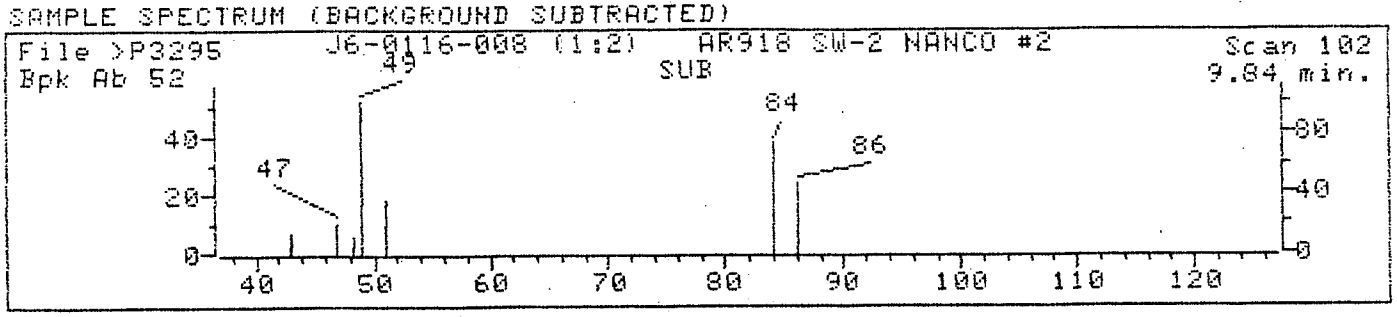

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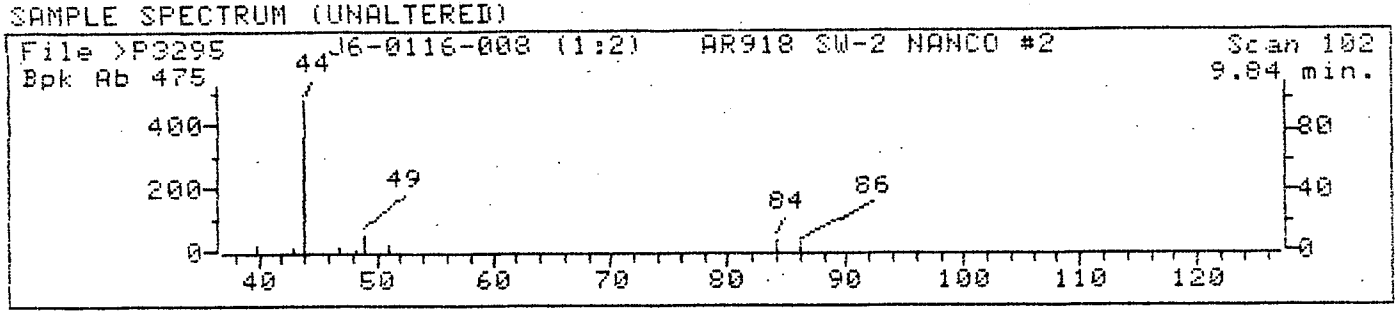
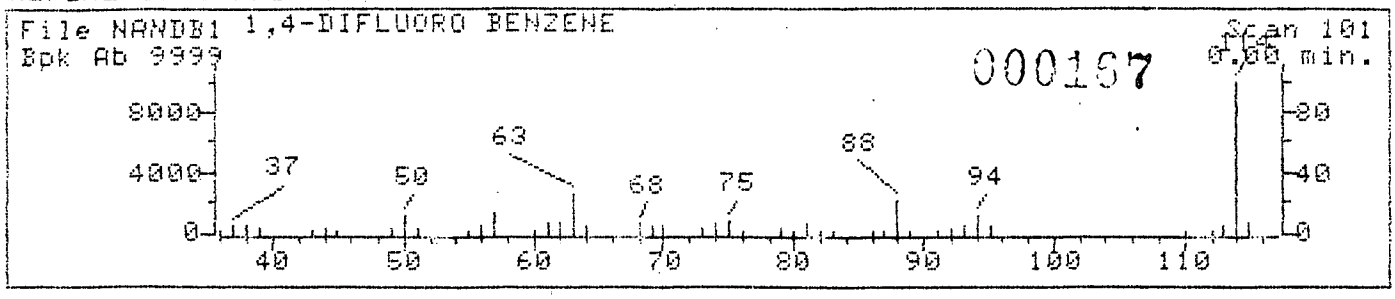


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

Compound No: 6
Compound Name: Methylene Chloride
Scan Number: 102
Retention Time: 9.84 min.
Area: 516
Concentration: 3.59 UG
a-value: 87

plg

REFERENCE STANDARD



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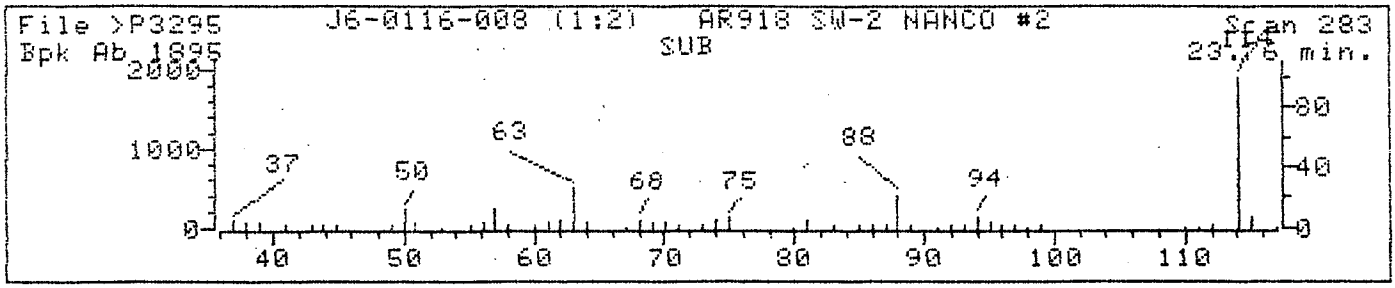
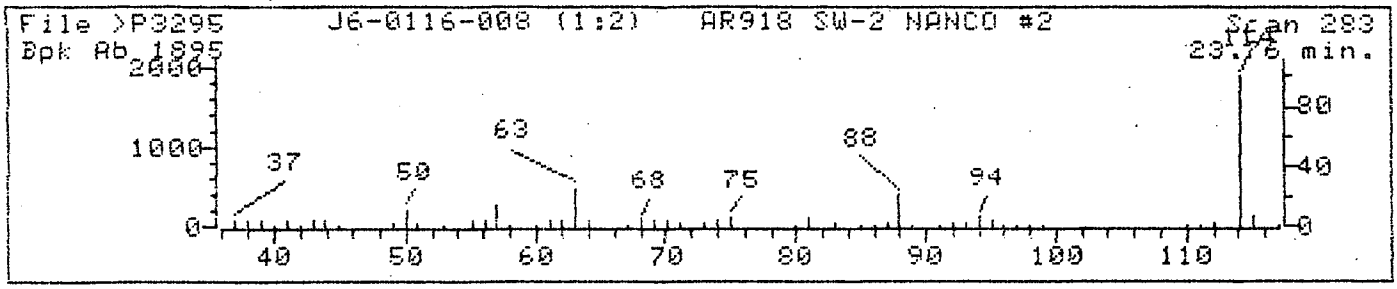


SAMPLE SPECTRUM (UNALTERED)

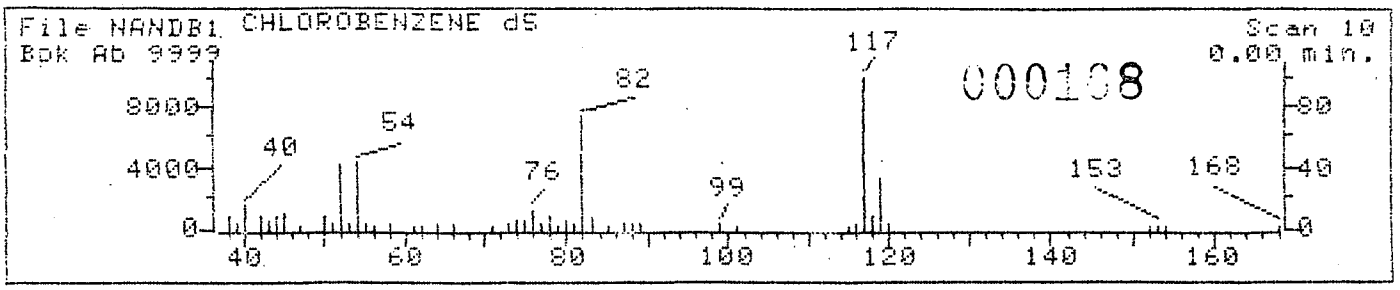


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

Compound No: 14 (ISTD)
Compound Name: 1,4-DIFLUOROBENZENE (ISTD)
Scan Number: 283
Retention Time: 23.76 min.
Area: 26282
Concentration: 50.00 UG
q-value: 96

plg

REFERENCE STANDARD SPECTRUM



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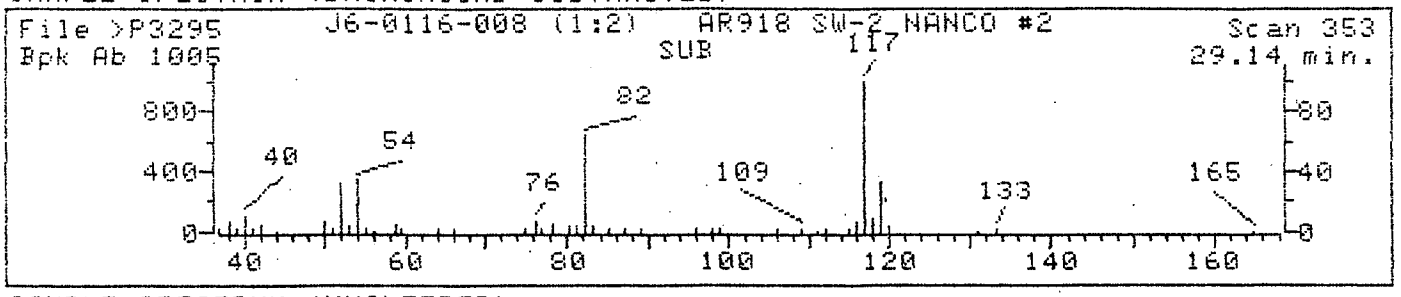

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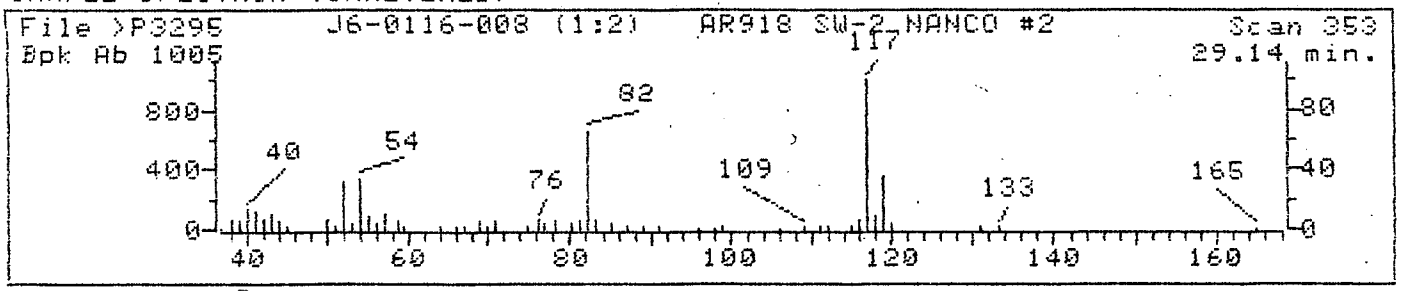
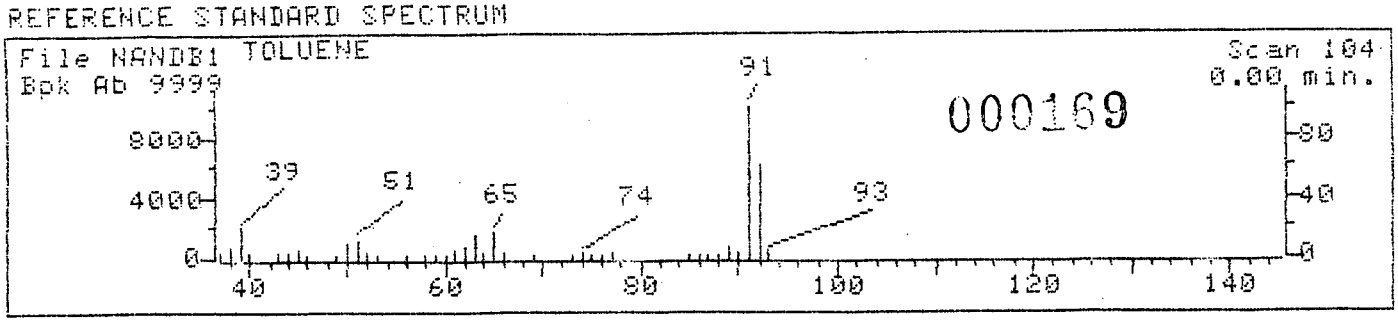


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

Compound No: 29 (ISTD)
Compound Name: CHLOROBENZENE-d5 (ISTD)
Scan Number: 353
Retention Time: 29.14 min.
Area: 18952
Concentration: 50.00 UG
a-value: 94

plg

REFERENCE STANDARD SPECTRUM



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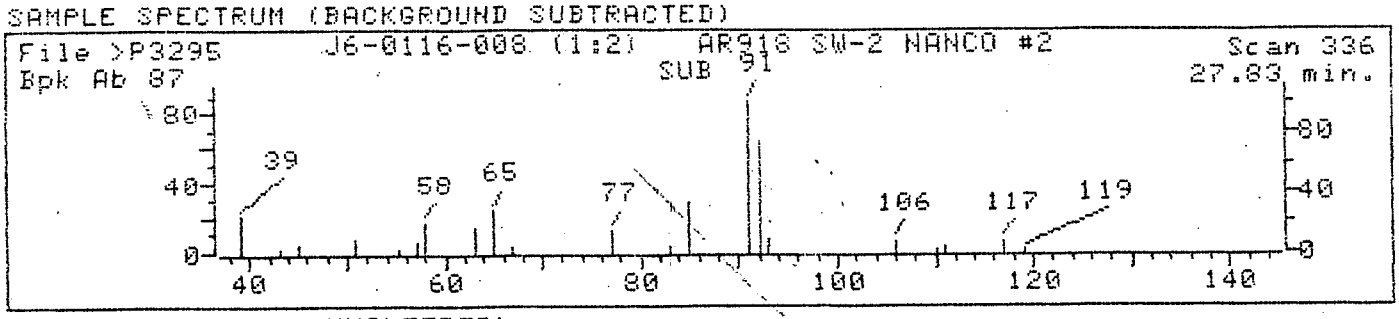
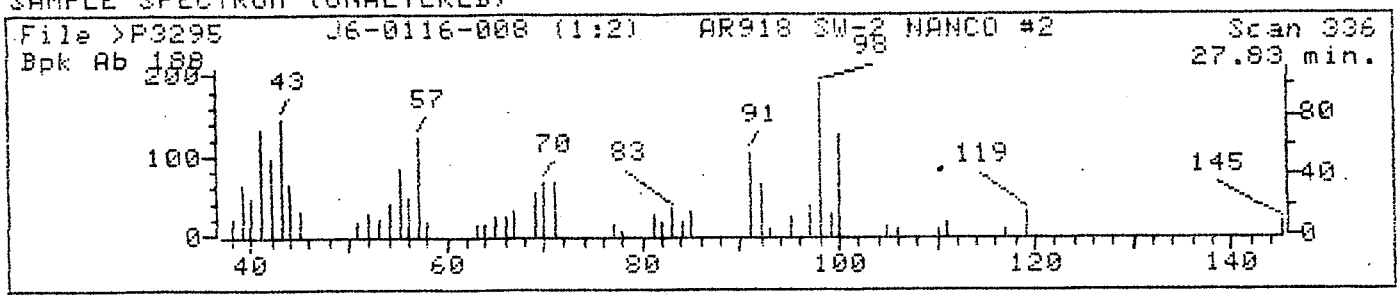


SAMPLE SPECTRUM (UNALTERED)

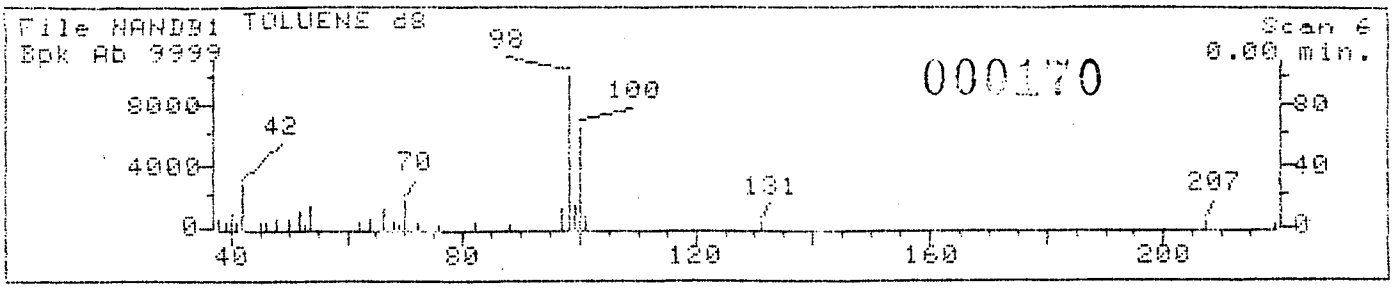


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

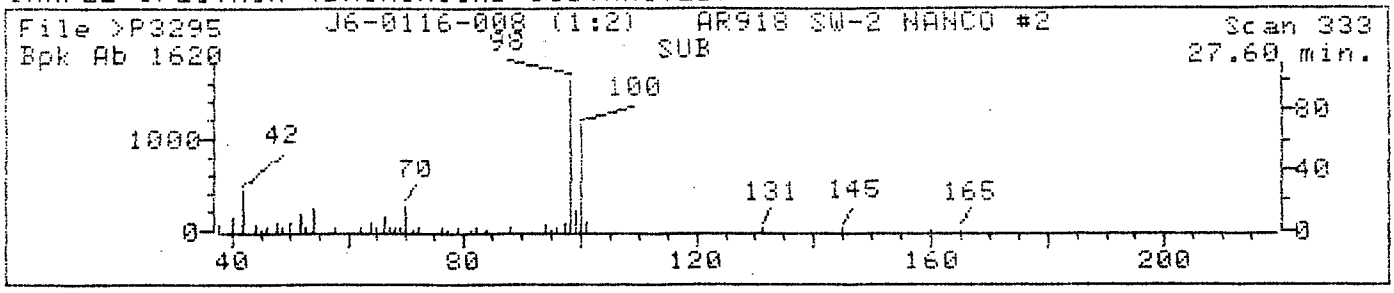
Compound No: 34
Compound Name: Toluene
Scan Number: 336
Retention Time: 27.83 min.
Area: 881
Concentration: 3.82 UG
a-value: 82

plg

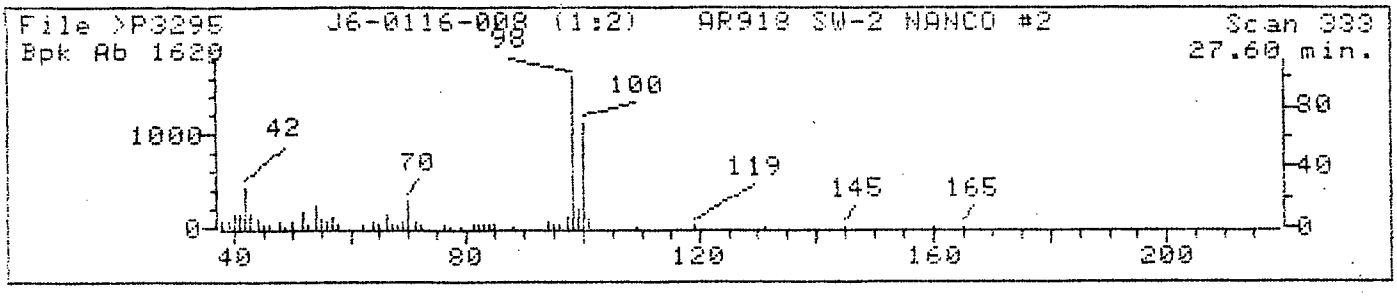
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)

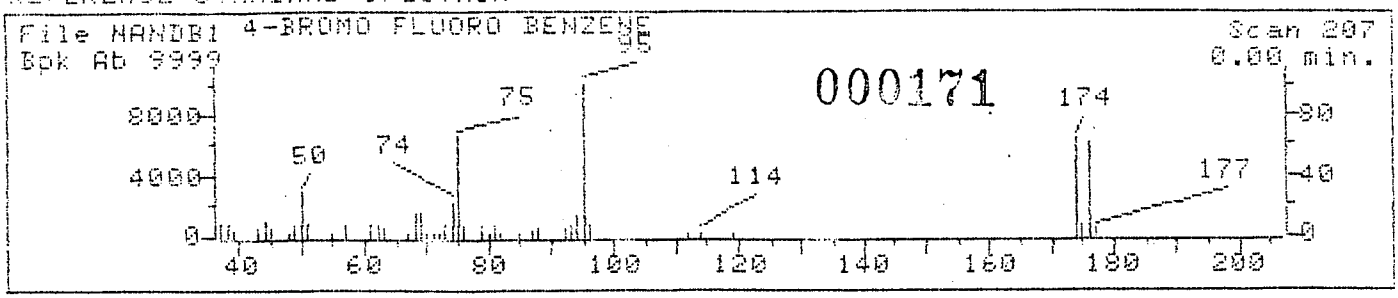


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

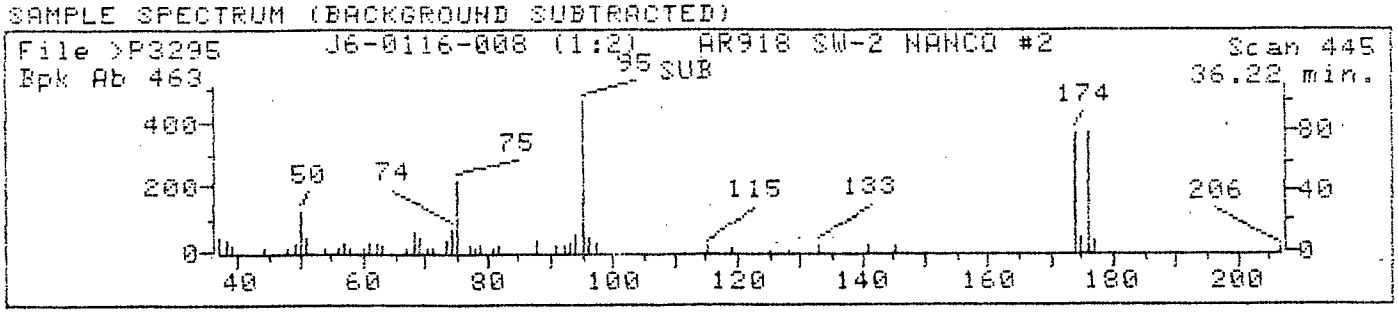
Compound No: 39
Compound Name: TOLUENE-d8 (a Surrog.)
Scan Number: 333
Retention Time: 27.60 min.
Area: 25794
Concentration: 98.84 UG
q-value: 97

plg

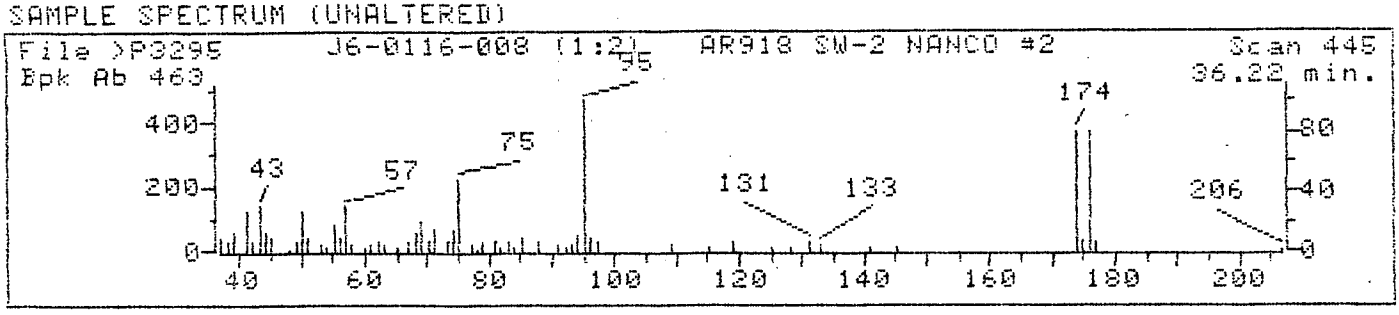
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)

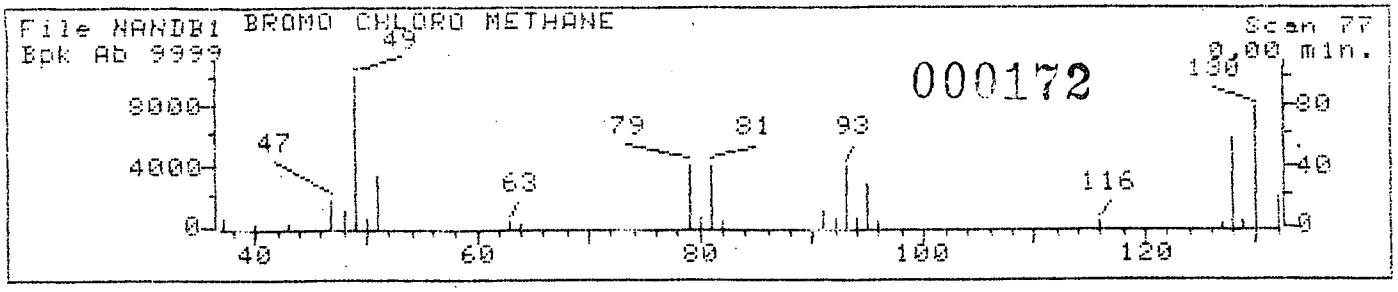


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

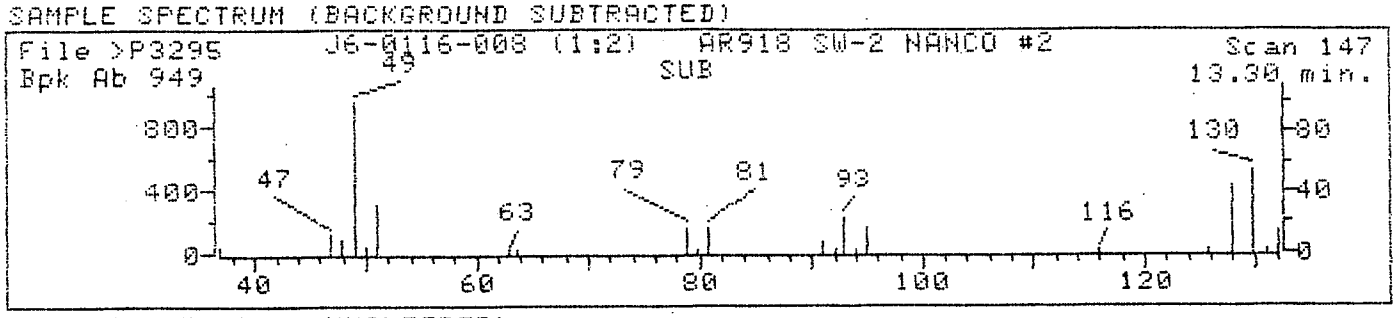
Compound No: 40
Compound Name: 4-BROMOFLUOROBENZENE (a Surrg)
Scan Number: 445
Retention Time: 36.22 min.
Area: 18154
Concentration: 107.72 UG
q-value: 87

pl9

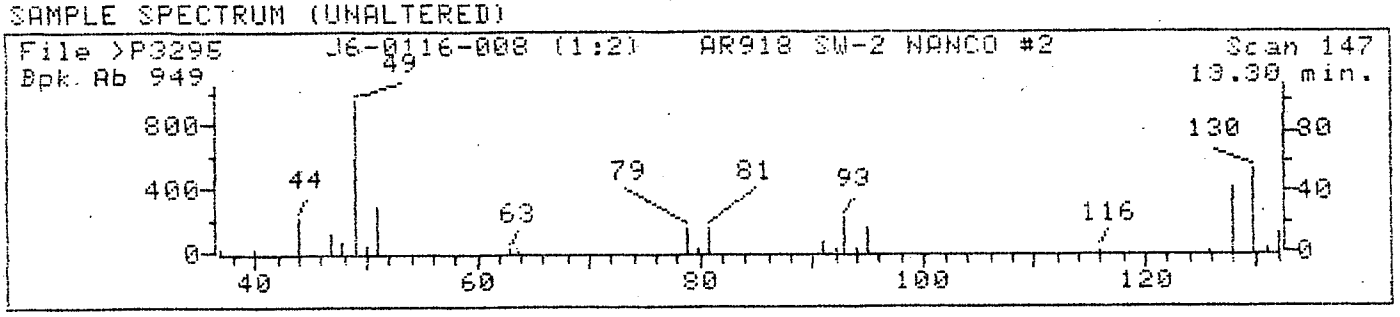
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)

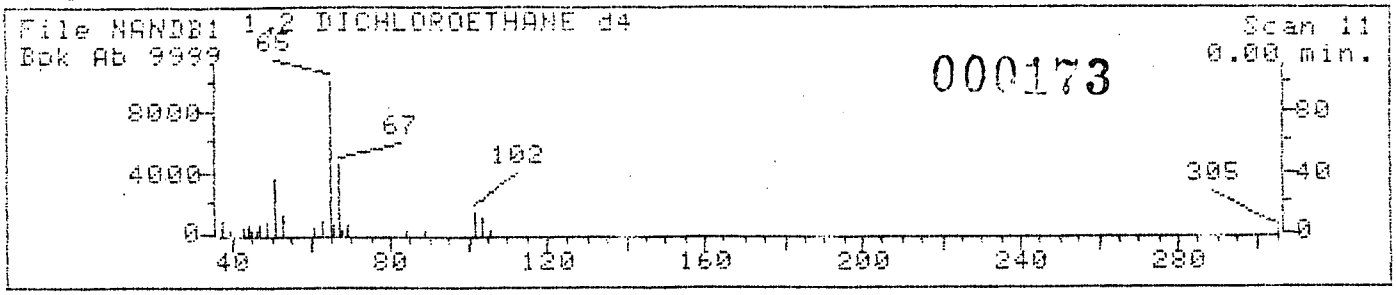


Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

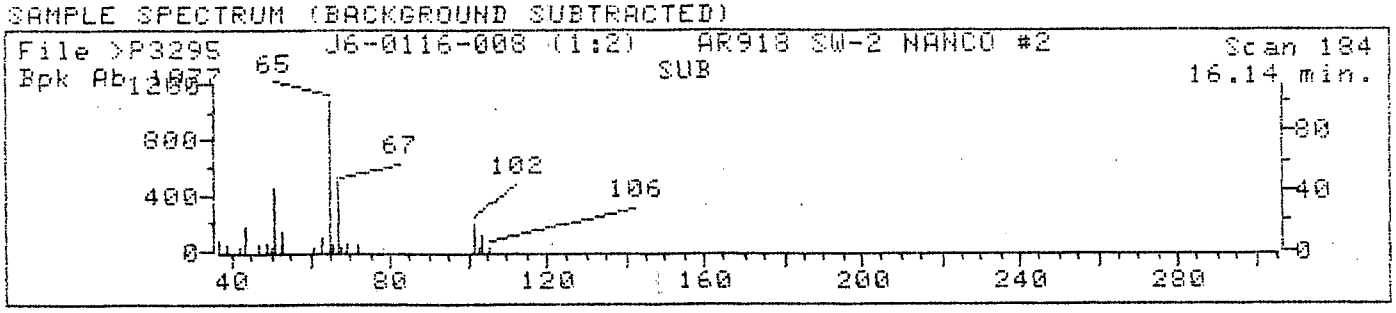
Compound No: 41 (ISTD)
Compound Name: [BROMOCHLOROMETHANE (ISTD)]
Scan Number: 147
Retention Time: 13.30 min.
Area: 5809
Concentration: 50.00 UG
q-value: 68

plg

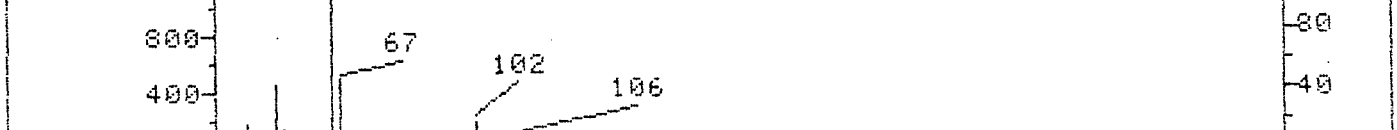
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



Data File: >P3295::D2
Name: J6-0116-008 (1:2)
Misc: AR918 SW-2 NANCO #2
Quant Time: 860923 10:35
Injected at: 860923 09:46

Compound No: 42
Compound Name: 1,2-DICHLOROETHANE-d4 (Surrog)
Scan Number: 184
Retention Time: 16.14 min.
Area: 14038
Concentration: 94.48 UG
a-value: 96

pls

MS data file header from : >P3295

000174

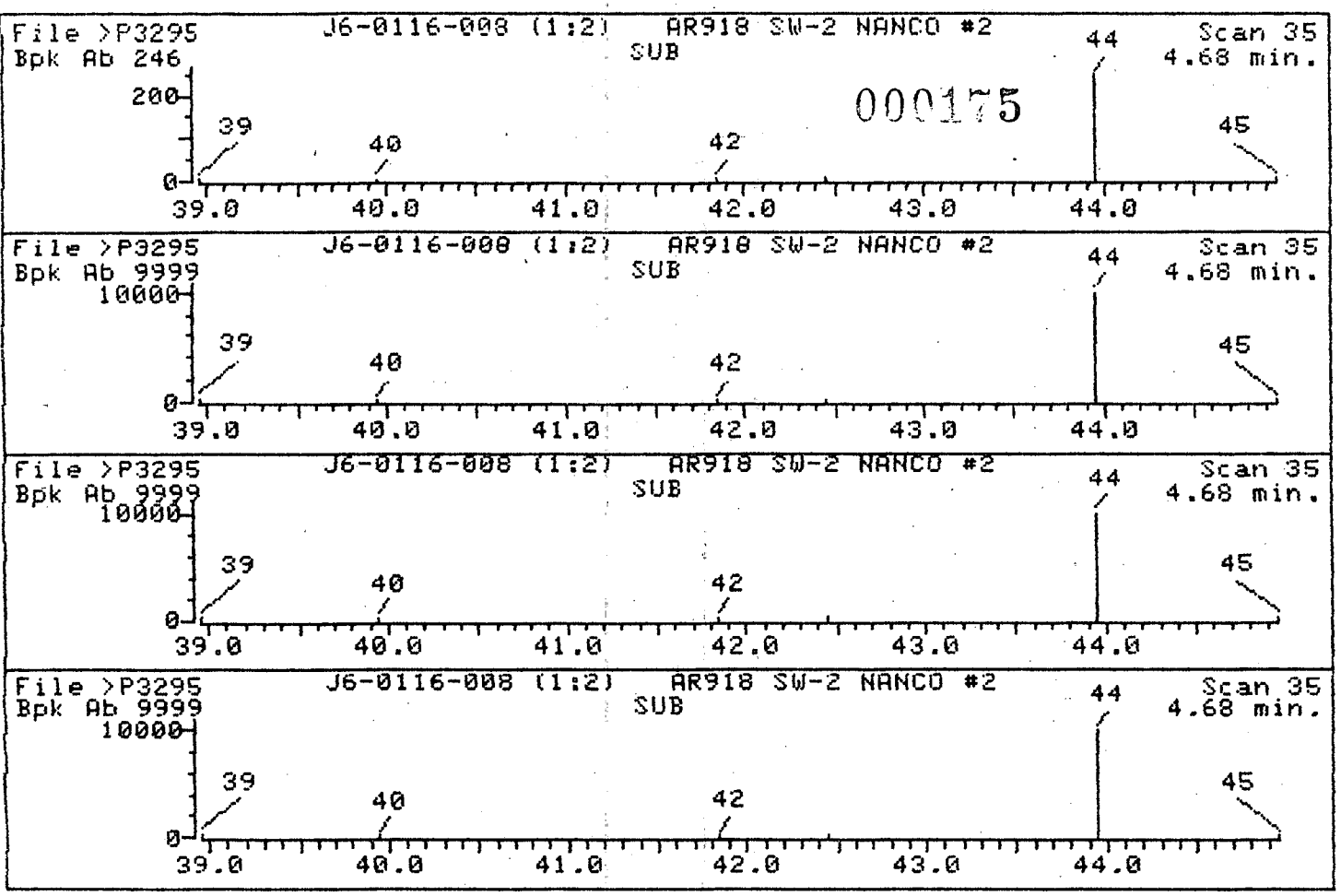
Sample: J6-0116-008 (1:2) Operator: DALY MS 9/23/86 9:46
Misc : AR918 SW-2 NANCO #2
Sys. #: 2 MS model: 96 SW/HW rev.: IA ALS # : 0
Method file: METH03 Tuning file: MT9002 No. of extra records: 1
Source temp.: 165 Analyzer temp.: 180 Transfer line temp. : 200

Chromatographic temperatures :	45.	220.	0.	0.	0.
Chromatographic times, min. :	4.0	22.0	0.0	0.0	0.0
Chromatographic rate, deg/min:	8.0	0.0	0.0	0.0	0.0

>P3295 J6-0116-008 (1:2) AR918 SW-2 NANCO #2
35.01 260.0 TIC

Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
	4.683	33	35	36	273	15752	3405	3.69	.776
2H	9.835	100	102	105	198	12794	2528	2.74	.576
	10.374	107	109	114	127	14894	2394	2.60	.545
1S4	13.296	143	147	157	3395	59107	46574	50.51	10.608
SU5	16.141	178	184	189	3098	47546	41201	44.68	9.384
	18.833	216	219	224	148	5126	2081	2.26	.474
	20.755	240	244	246	149	4319	2297	2.49	.523
	21.140	246	249	256	251	10788	5943	6.44	1.354
9	22.832	266	271	274	400	14768	7716	8.37	1.757
1S10	23.755	279	283	287	5038	89867	75500	81.88	17.196
	24.909	295	298	299	147	13825	2303	2.50	.525
	25.371	302	304	306	228	15141	2880	3.12	.656
	27.294	326	329	329	322	19401	3558	3.86	.810
SU14	27.602	329	333	342	5327	153911	92213	100.00	21.003
1S15	29.141	348	353	361	3598	137208	70526	76.48	16.063
SU16	36.220	438	445	454	2250	167550	77936	84.52	17.751

Sum of corrected areas: 439055.



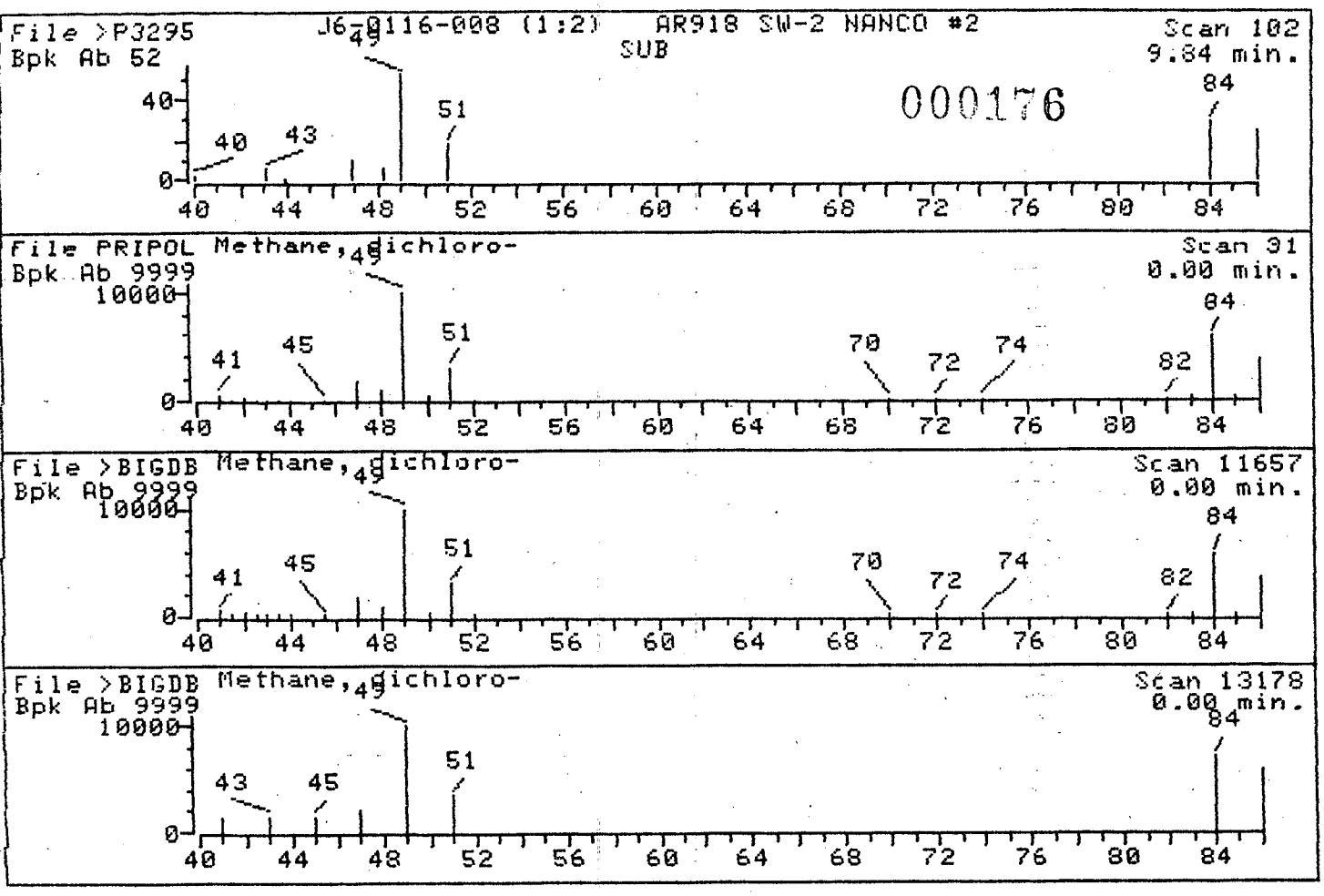
000175

<10% IS

Sample file: >P3295 Spectrum #: 35

No data base entries were retrieved.

plg



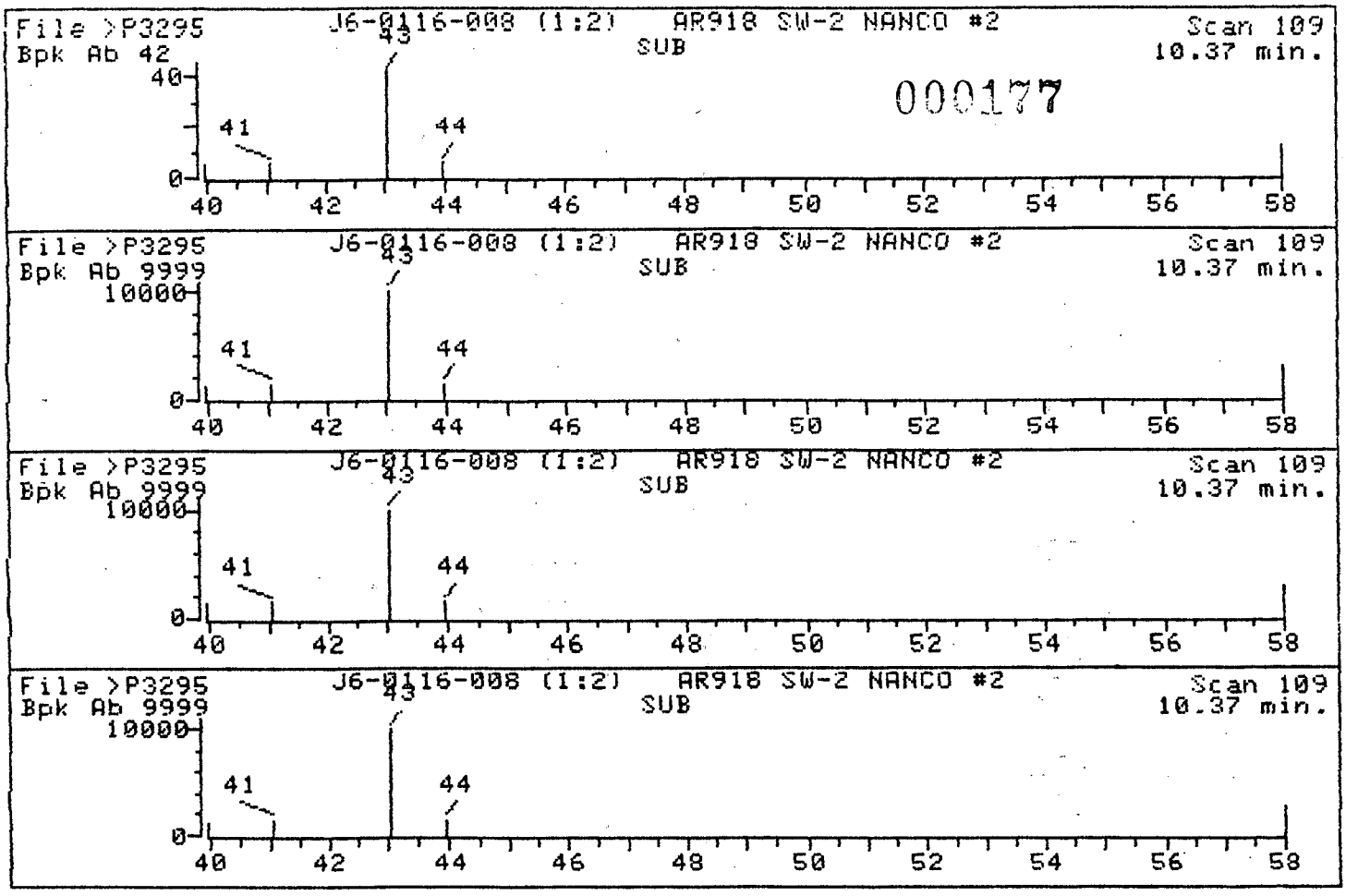
1. Methane, dichloro- 84 CH2Cl2
2. Methane, dichloro- 84 CH2Cl2
3. Methane, dichloro- 84 CH2Cl2
4. Methane, dichloro- 84 CH2Cl2
5. Methane, dichloro- 84 CH2Cl2

HSL

plg

Sample file: >P3295 Spectrum #: 102
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	79*	31	112	PRIPOL	55	48	2	0	96	8	48	32
2.	79*	75092	11657	"BIGDB	55	48	2	0	96	8	48	32
3.	76*	75092	13178	"BIGDB	53	27	3	0	78	8	45	25
4.	76*	32	128	PRIPOL	53	27	3	0	78	8	45	25
5.	67*	75092	13177	"BIGDB	47	52	2	0	87	13	34	21



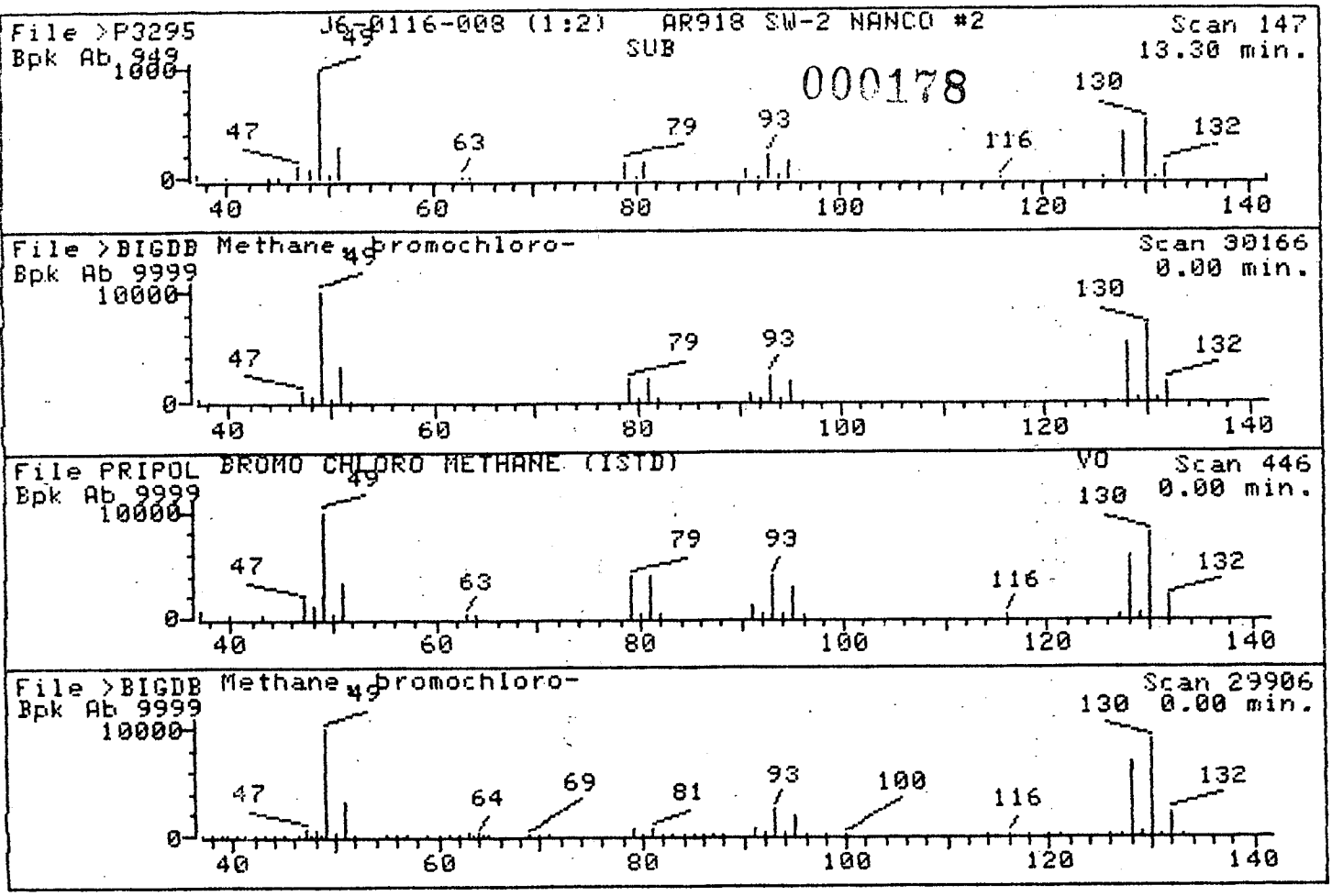
000177

<10% IS

Sample file: >P3295 Spectrum #: 109

No data base entries were retrieved.

pls



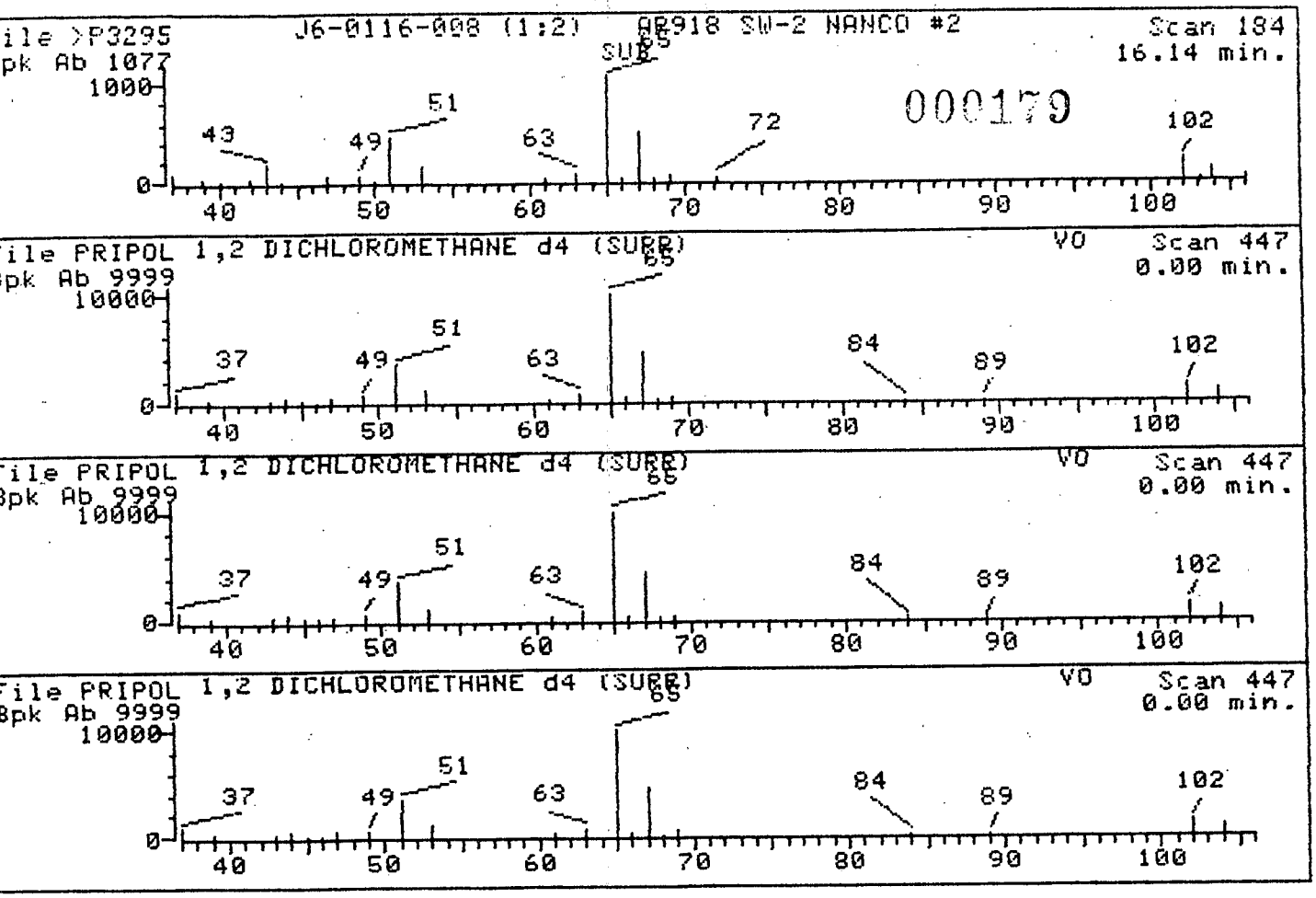
000178

1. Methane, bromochloro- 128 CH2BrCl
2. BROMO CHLORO METHANE (ISTD) VO 128 CH2BrCl
   A INTERNAL STANDARD
3. Methane, bromochloro- 128 CH2BrCl

plg

Sample file: >P3295 Spectrum #: 147
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	96*	74975	30166	"BIGDB	101	12	1	0	80	4	72	94
2.	79*	446	204	PRIPOL	68	43	0	0	39	36	37	83
3.	45*	74975	29906	"BIGDB	50	62	2	0	60	27	19	23



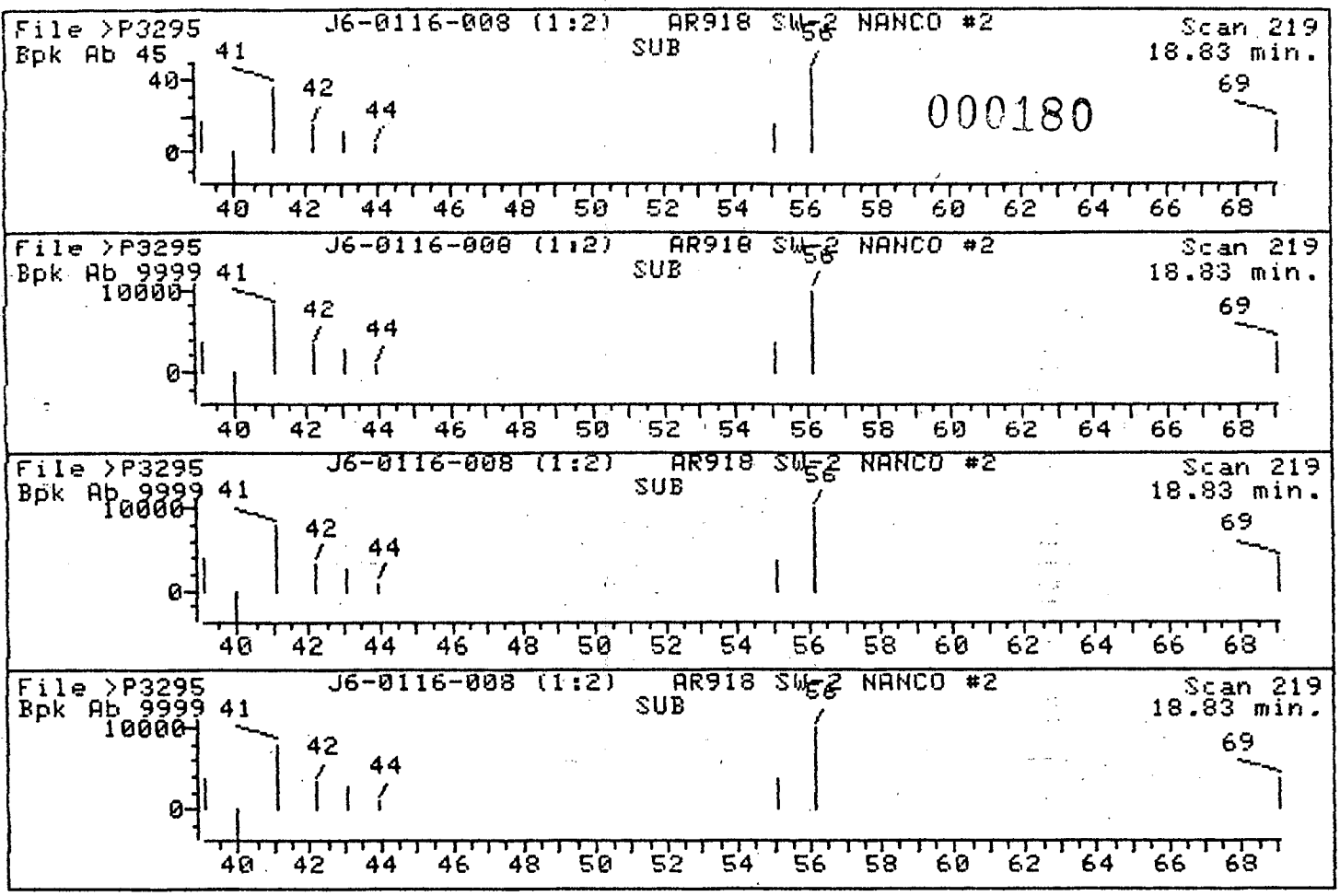
000179

1. 1,2 DICHLOROMETHANE d4 (SURR) VO 102
LATILE SURROGATE

plg

Sample file: >P3295 Spectrum #: 184
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	86*	447	64	PRIPOL	59	41	2	0	99	1	60	36



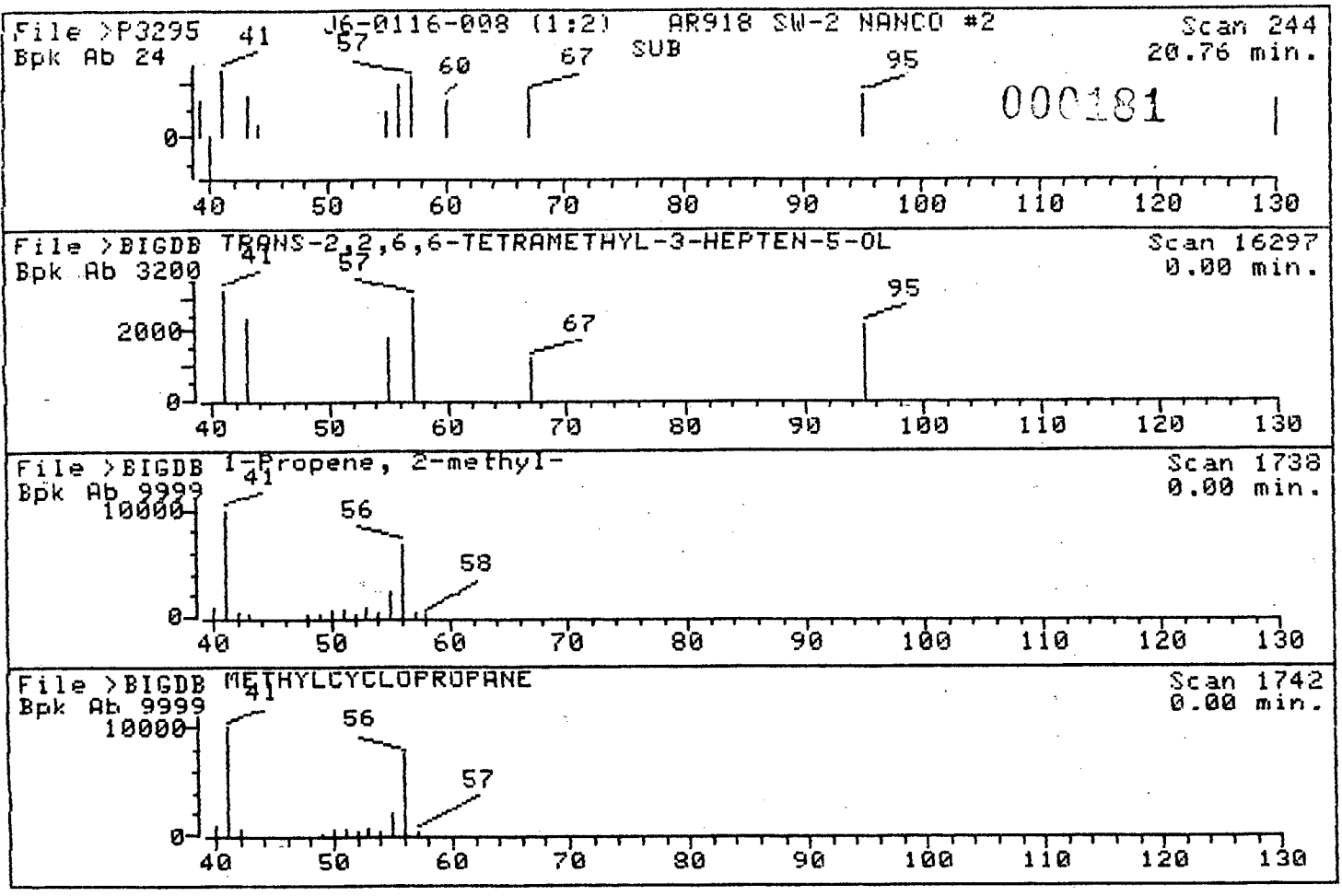
000180

<10% IS

Sample file: >P3295 Spectrum #: 219

pls

No data base entries were retrieved.



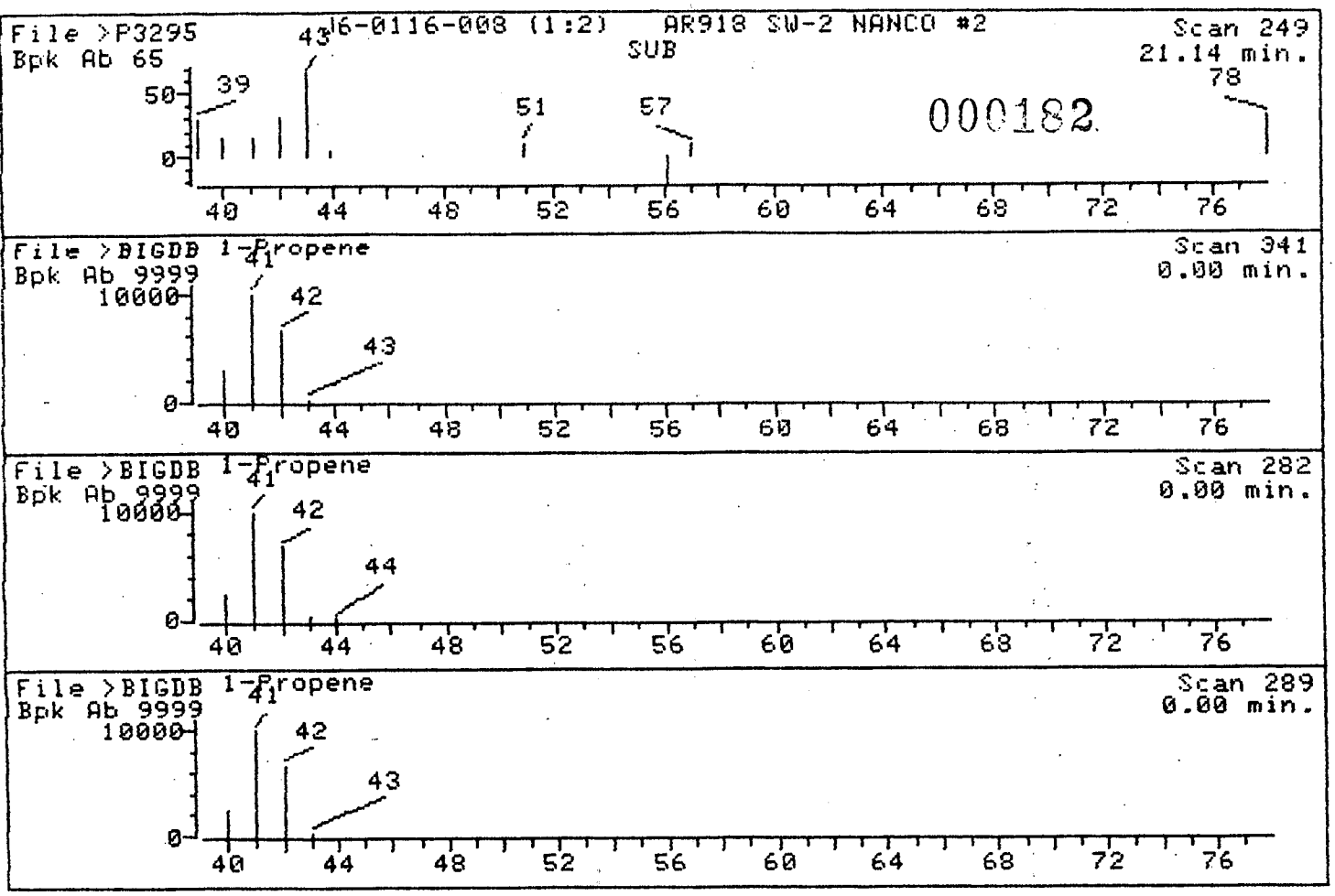
<10% IS

1. TRANS-2,2,6,6-TETRAMETHYL-3-HEPTEN-5-OL 170 C11H220
2. 1-Propene, 2-methyl- 56 C4H8
3. METHYLCYCLOPROPANE 56 C4H8

pls

Sample file: >P3295 Spectrum #: 244
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	25	0	16297	"BIGDB	36	31	1	0	66	45	8	13
2.	20*	115117	1738	"BIGDB	21	60	2	0	100	53	5	13
3.	20*	0	1742	"BIGDB	22	65	2	0	100	53	5	13



1. 1-Propene
2. 1-Propene
3. 1-Propene
4. 1-Propene

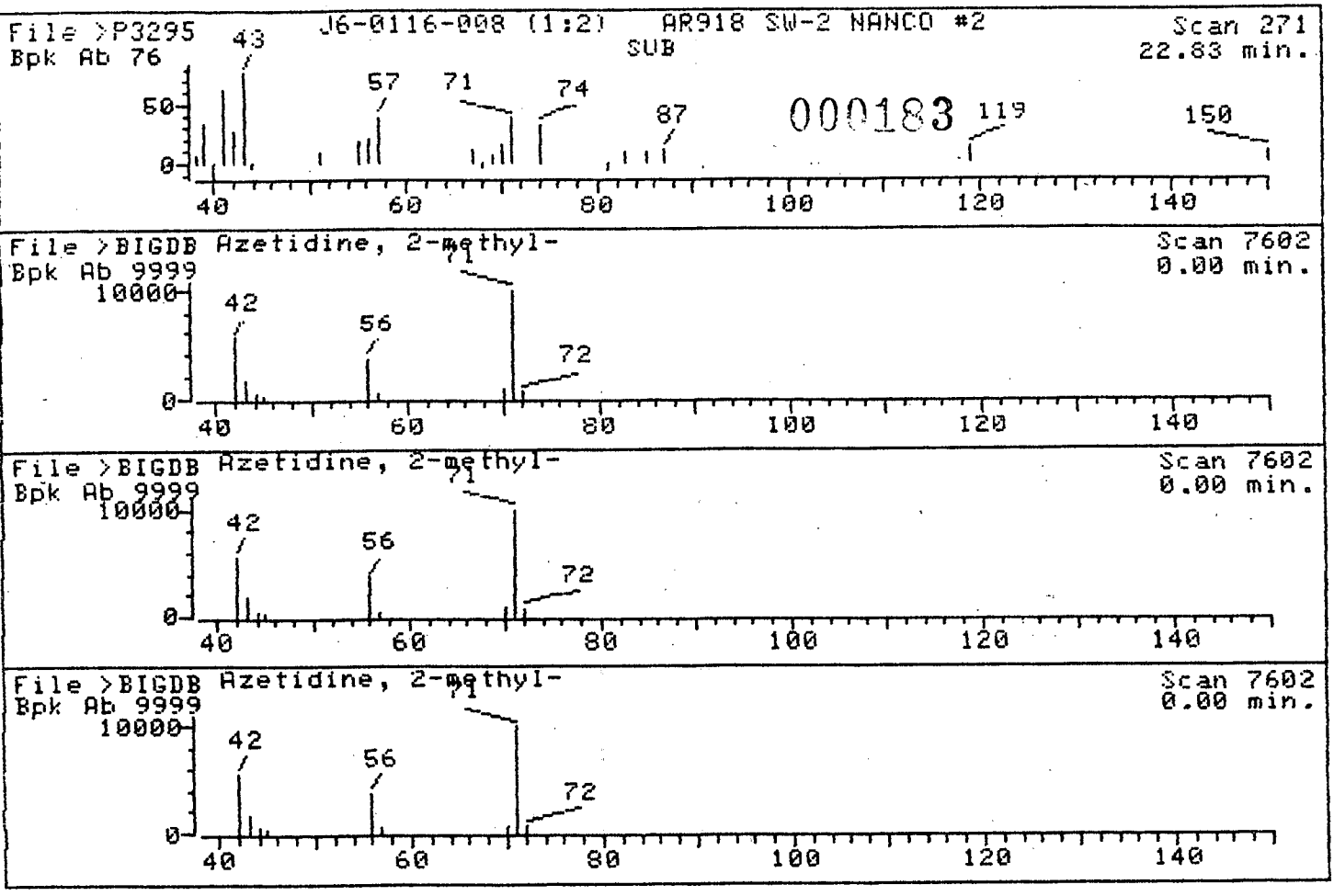
<10% IS

plg

42 C3H6
42 C3H6
42 C3H6
42 C3H6

Sample file: >P3295 Spectrum #: 249
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	11*	115071	341	"BIGDB	25	56	1	0	57	61	2	14
2.	11*	115071	282	"BIGDB	22	62	1	0	68	61	2	14
3.	11*	115071	289	"BIGDB	22	68	1	0	64	61	2	14
4.	11*	115071	304	"BIGDB	22	73	1	0	61	62	2	14



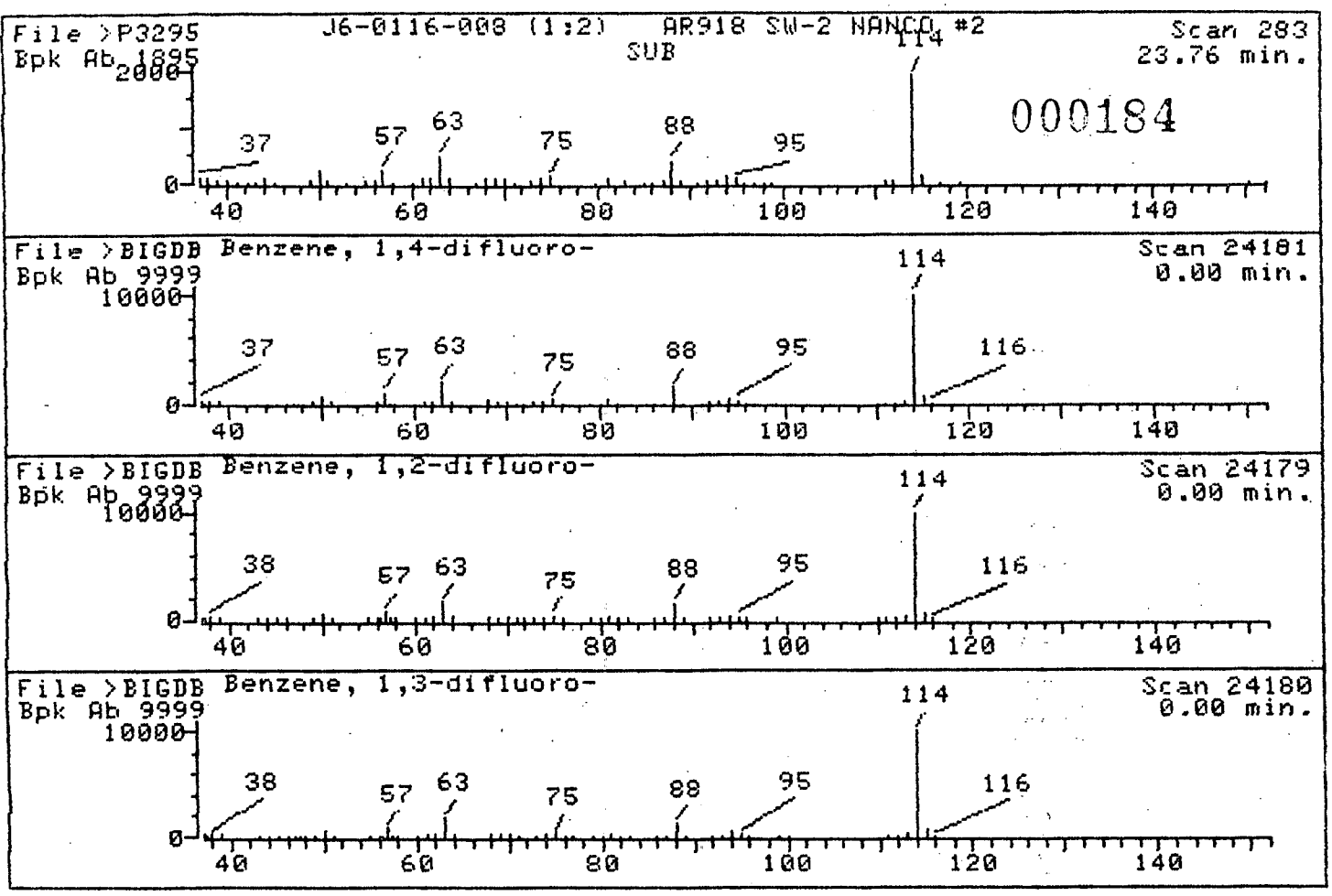
1. Azetidine, 2-methyl- 71 C4H9N

plg

Sample file: >P3295 Spectrum #: 271

Search speed: 1 Tilting option: N No. of ion ranges searched: 46

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	11*	19812498	7602	"BIGDB	21	31	2	0	48	61	2	13



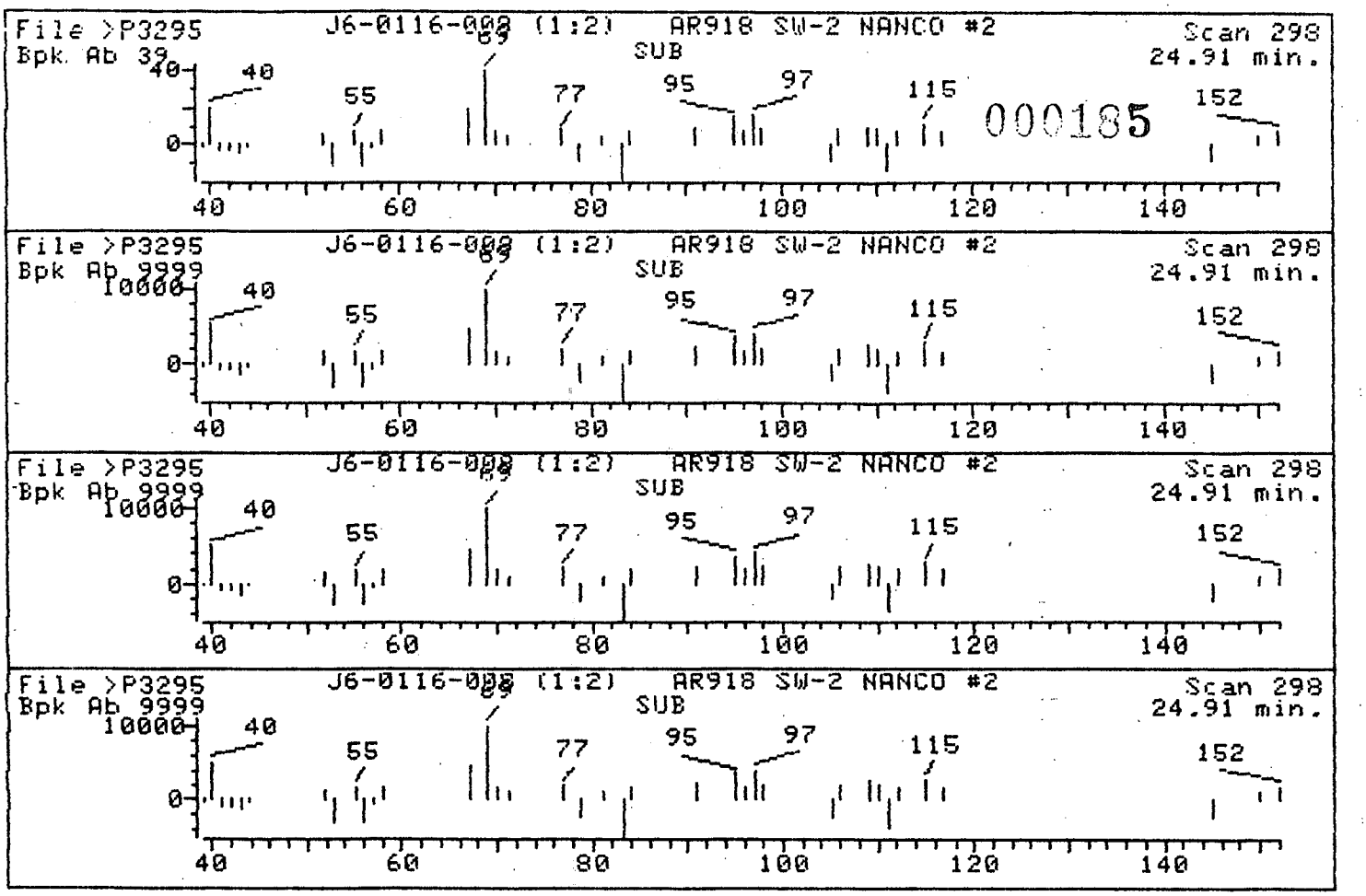
000184

1. Benzene, 1,4-difluoro- I.S. 114 C6H4F2
2. Benzene, 1,2-difluoro- 114 C6H4F2
3. Benzene, 1,3-difluoro- 114 C6H4F2
4. Benzene, 1,4-difluoro- 114 C6H4F2

plg

Sample file: >P3295 Spectrum #: 283
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	96*	540363	24181	"BIGDB	84	5	1	0	100	0	72	96
2.	89*	367113	24179	"BIGDB	65	20	1	0	100	1	66	73
3.	86*	372189	24180	"BIGDB	67	18	1	0	100	6	59	77
4.	64*	540363	24611	"BIGDB	51	30	1	0	88	24	28	43



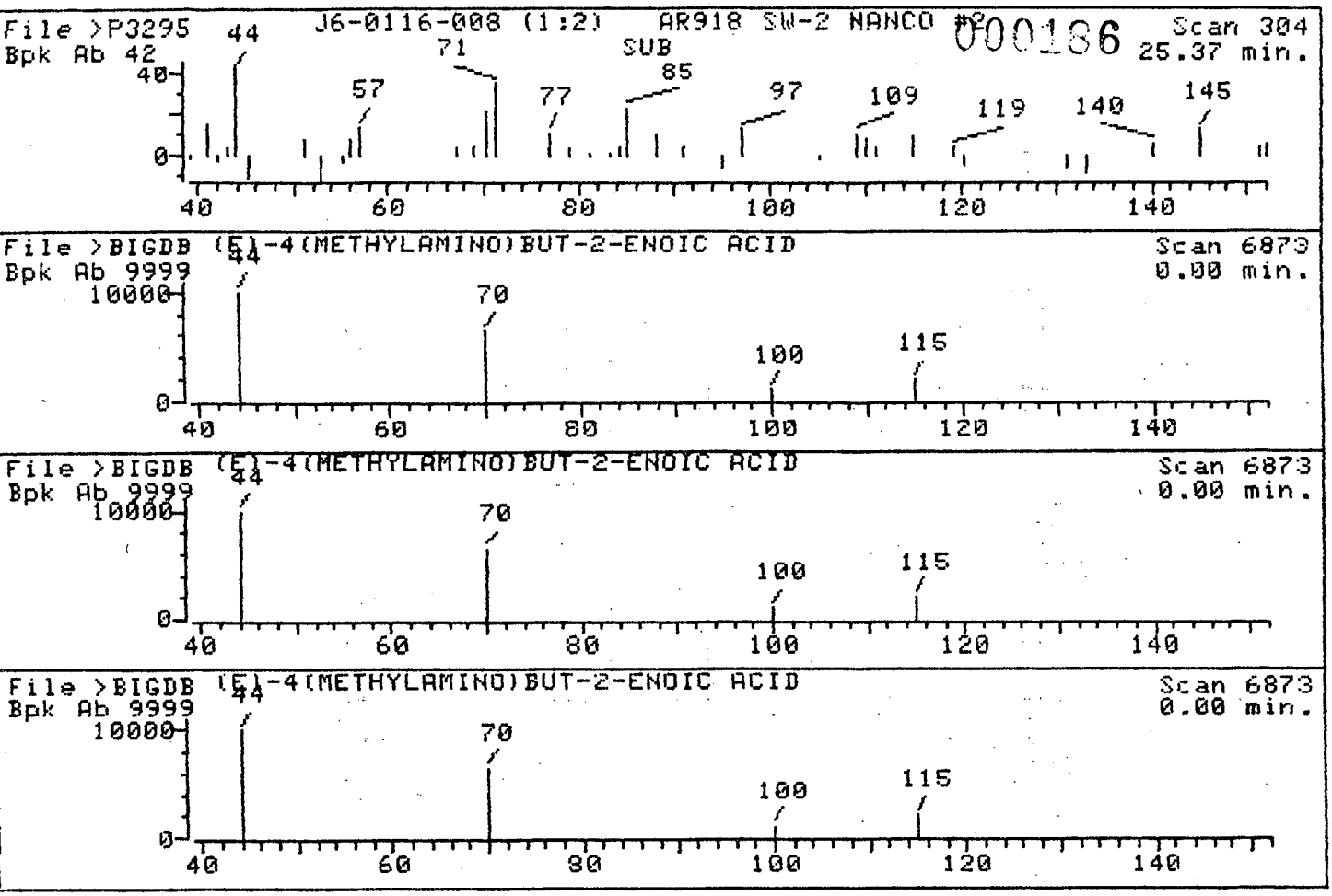
000185

<10% IS

Sample file: >P3295 Spectrum #: 298

No data base entries were retrieved.

plg



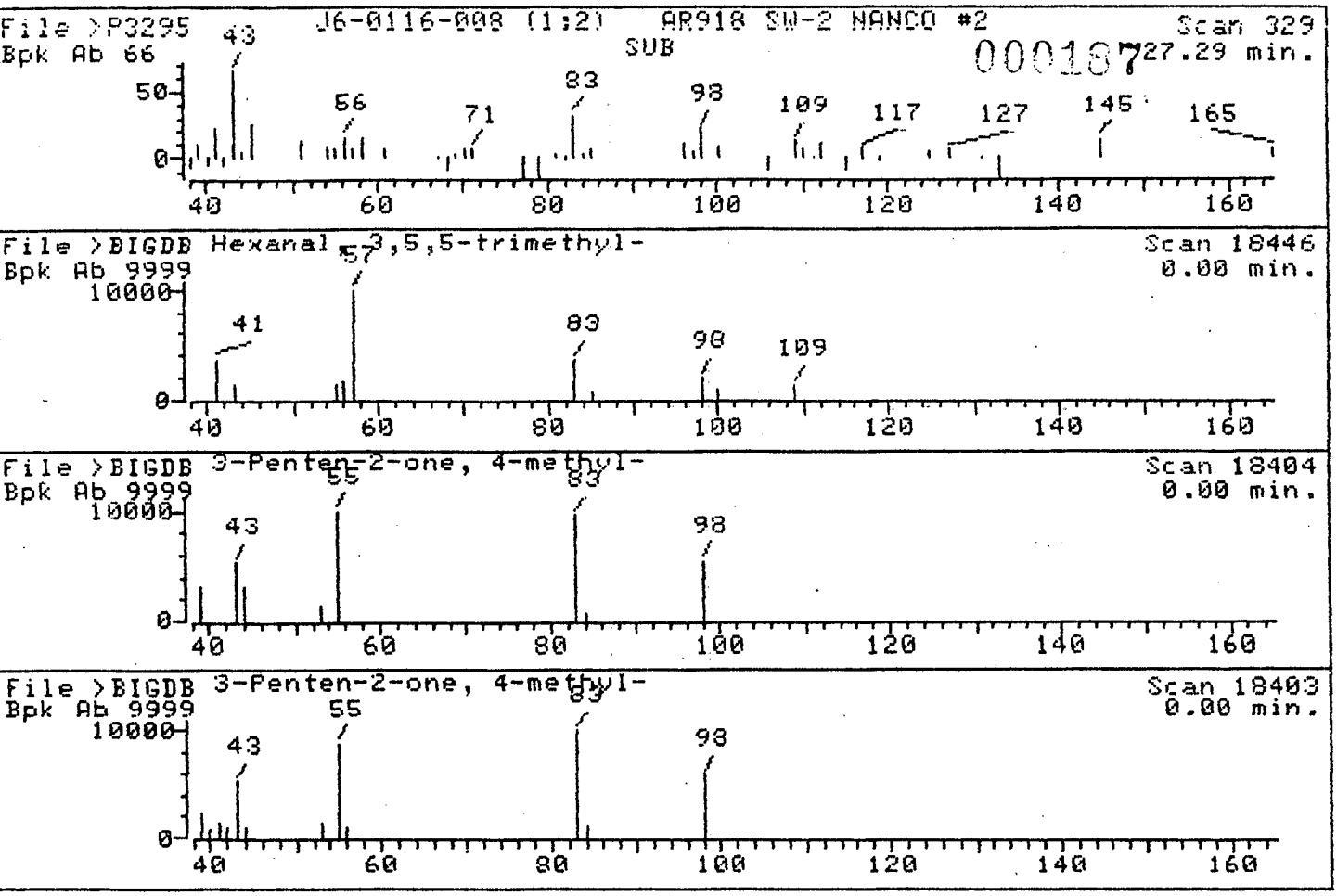
<10% IS

plg

1. (E)-4(METHYLAMINO)BUT-2-ENOIC ACID 115 C5H9NO2

Sample file: >P3295 Spectrum #: 304
Search speed: 1 Tilting option: N No. of ion ranges searched: 47

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	11*	0	6873	"BIGDB	24	8	1	0	77	65	2	14



000187

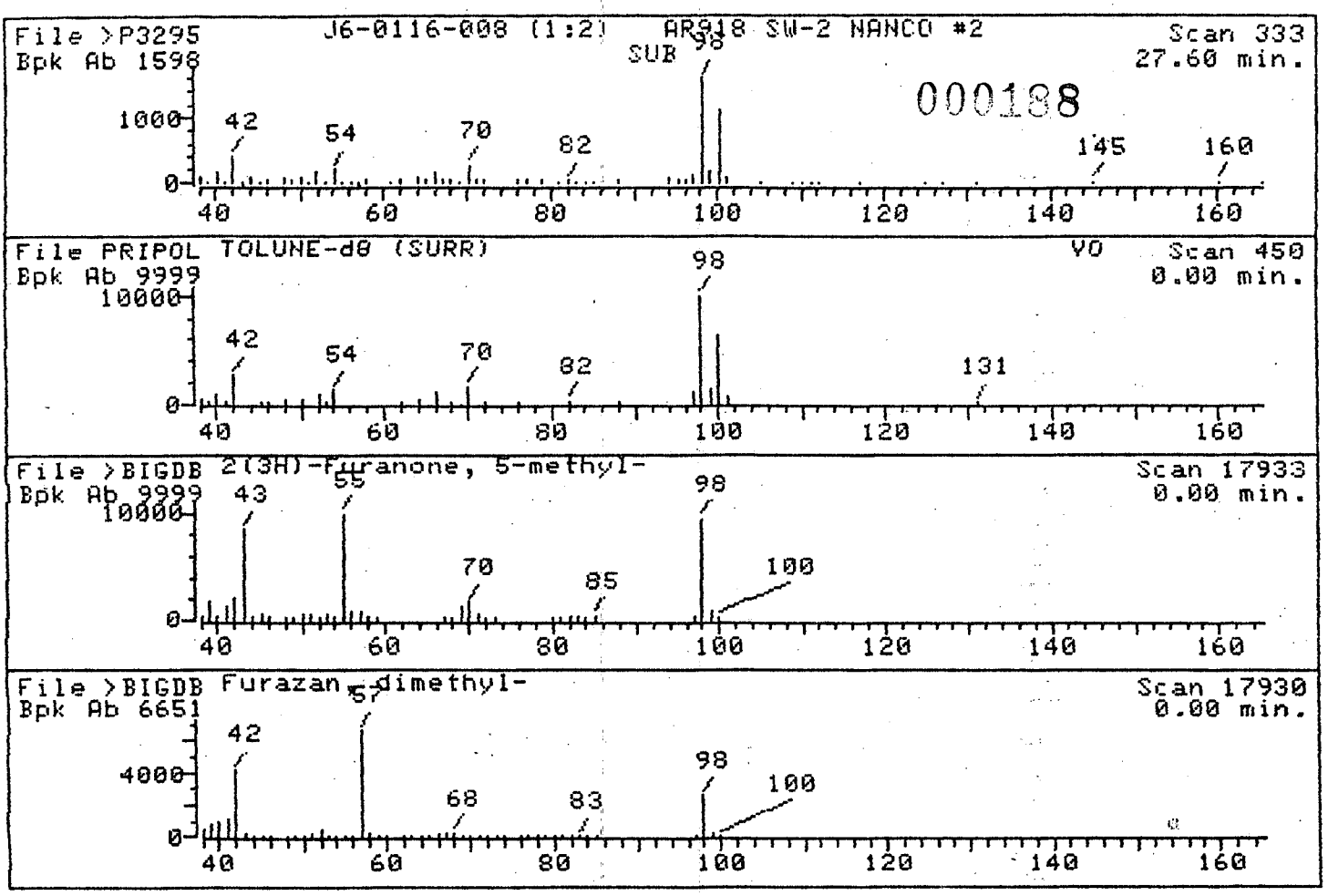
<10% IS

1. Hexanal, 3,5,5-trimethyl- 142 C9H18O
2. 3-Penten-2-one, 4-methyl- 98 C6H10O
3. 3-Penten-2-one, 4-methyl- 98 C6H10O
4. 1H-Pyrazole, 4,5-dihydro-4,5-dimethyl- 98 C5H10N2
5. Furan, 2,5-dihydro-2,5-dimethyl- 98 C6H10O

plg

Sample file: >P3295 Spectrum #: 329
Search speed: 1 Tilting option: N No. of ion ranges searched: 54

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	24	5435643	18446	"BIGDB	43	20	3	0	136	43	8	12
2.	11*	141797	18404	"BIGDB	24	36	2	0	45	62	2	14
3.	11*	141797	18403	"BIGDB	23	50	3	0	48	62	2	12
4.	11*	28019945	17944	"BIGDB	25	53	3	0	48	62	2	13
5.	11*	59242272	17966	"BIGDB	30	60	3	0	48	62	2	13

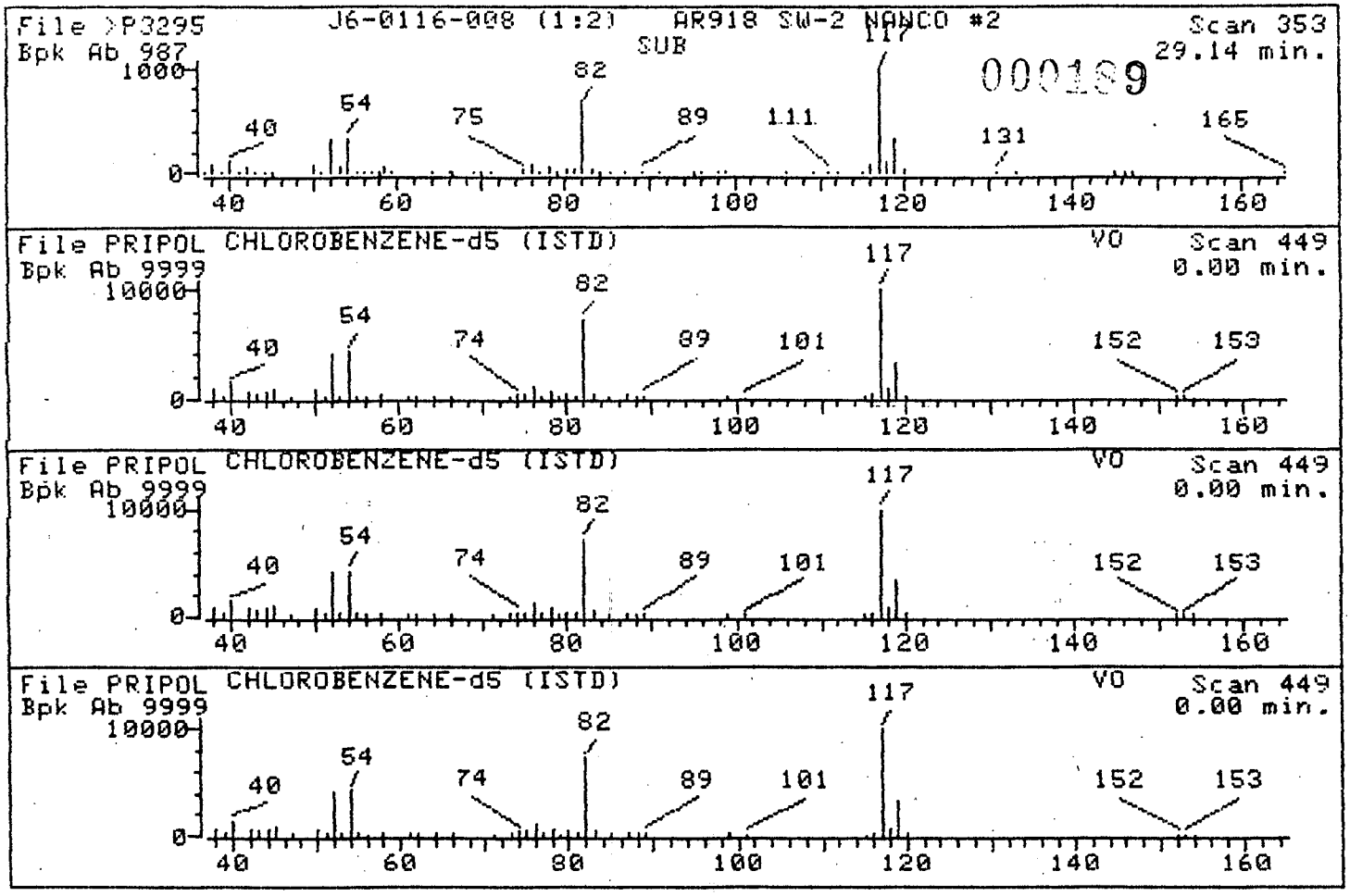


1. TOLUNE-d8 (SURR) VO 96
   LATILE SURROGATE
2. 2(3H)-Furanone, 5-methyl- 98 C5H6O2
3. Furazan, dimethyl- 98 C4H6N2O

pl9

Sample file: >P3295 Spectrum #: 333
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	44	450	158	PRIPOL	73	25	2	0	83	31	16	27
2.	30*	591128	17933	"BIGDB	27	73	3	0	105	31	12	13
3.	25*	4975217	17930	"BIGDB	22	69	2	0	270	47	7	13



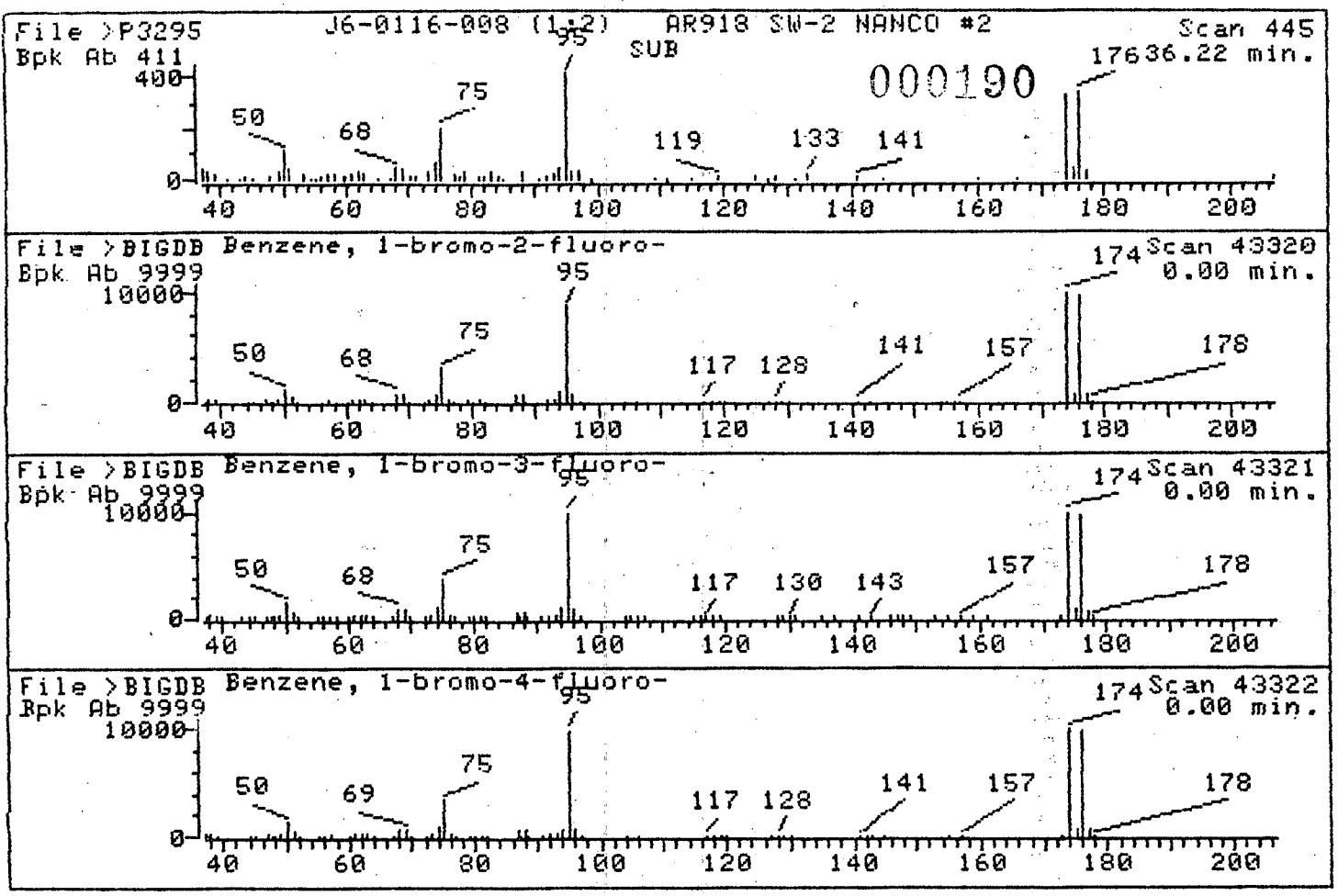
000189

1. CHLOROBENZENE-d5 (ISTD) VO 117
A INTERNAL STANDARD

plg

Sample file: >P3295 Spectrum #: 353
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	78*	449	177	PRIPOL	32	73	3	0	90	2	55	13



1. Benzene, 1-bromo-2-fluoro- 174 C6H4BrF
2. Benzene, 1-bromo-3-fluoro- 174 C6H4BrF
3. Benzene, 1-bromo-4-fluoro- 174 C6H4BrF
4. 4-BROMO FLUORO BENZENE SU 174 C6H4BrF
RROGATE COMPOUND

pls

Sample file: >P3295 Spectrum #: 445
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	74*	1072851	43320	"BIGDB	65	42	2	0	80	14	39	44
2.	74*	1073069	43321	"BIGDB	67	46	2	0	80	11	39	46
3.	71*	460004	43322	"BIGDB	60	50	2	0	80	12	38	37
4.	62*	451	144	PRIPOL	66	50	2	0	73	28	25	45

DJ DEP 4/23/86

1078

000191

Dil 1:2

>P3295 J6-0116-008 SW-2

HSL'S	CONC ug/l
Methylene Chloride	3.59 J
Toluene	3.82 JB

SURR'S		% REC
Tol d8	98.84	99
4BFB	107.72	108
1,2-Cl_2 ethane d4	94.48	95

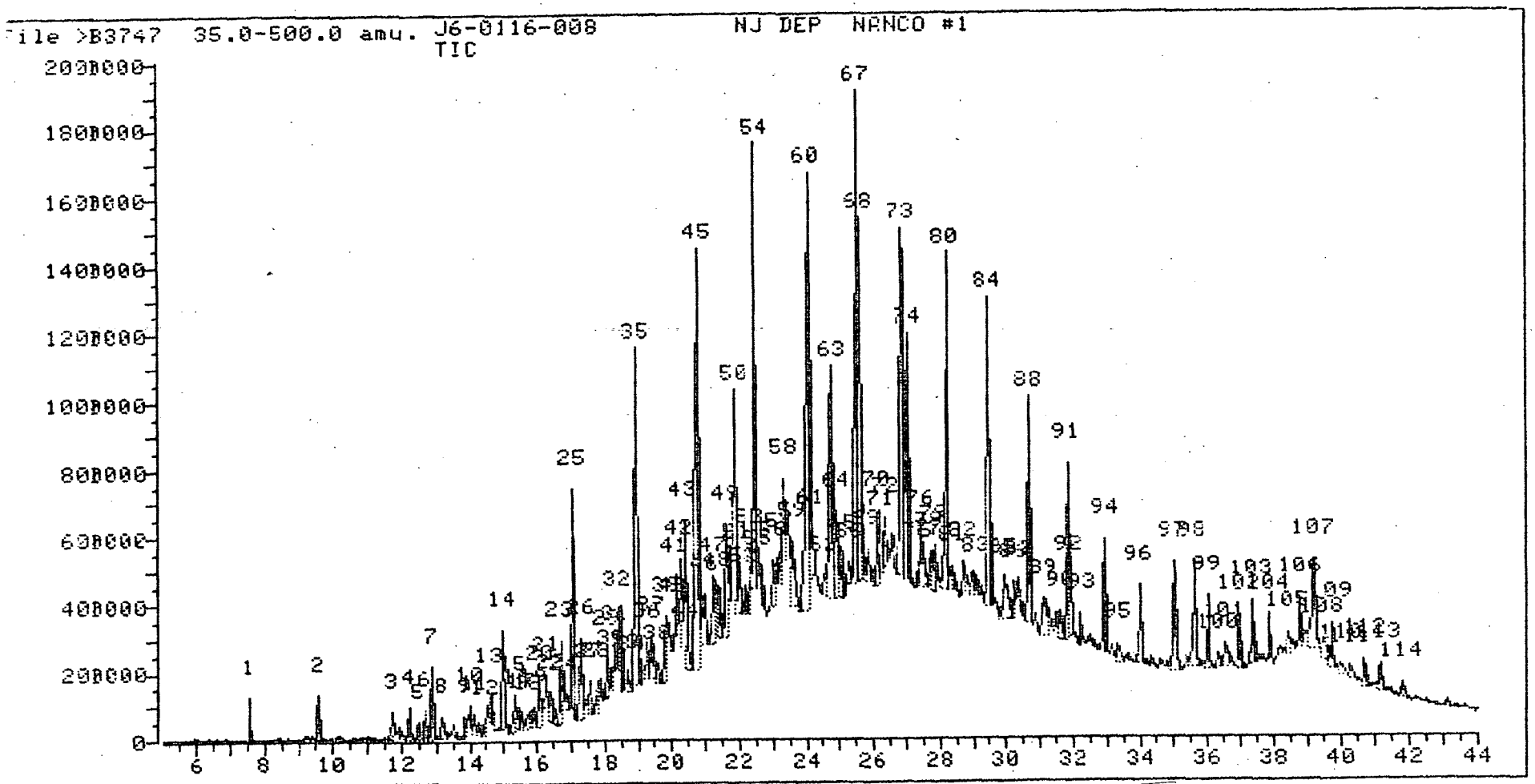
TIC'S

12498 2-METHYL AZETIDINE (22.83)

$x = (7716/75500) \times 50 = 5.1$ J

D. Nunnah 10/26/87

Inj: 10/22/86 1813



PK #		
7	1,4-DICHLOROBENZENE d4	(IS)
23	NAPHTHALENE d8	(IS)
53	ACENAPHTHENE d10	(IS)
73	PHENANTHRENE d10	(IS)
93	CHRYSENE d12	(IS)
107	PERYLENE d12	(IS)

PK #		
4	PHENOL d6	(SURR)
2	2-FLUOROPHENOL	(SURR)
13	NITROBENZENE d5	(SURR)
23	2-FLUOROBIPHENYL	(SURR)
42	2,4,6-TRIBROMOPHENOL	(SURR)
63	TERPHENYL d14	(SURR)

000102

QUANT REPORT

Operator ID: MORRIS
Output File: ^B3747::AQ
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1

Quant Rev: 4
Quant Time: 861023 09:57
Injected at: 861022 18:13
Dilution Factor: ~~74.00~~ 2.22 (50)

BTL# 3

ID File: IDEPA1::NA
Title: IDEPA BNA
Last Calibration: 861023 09:48

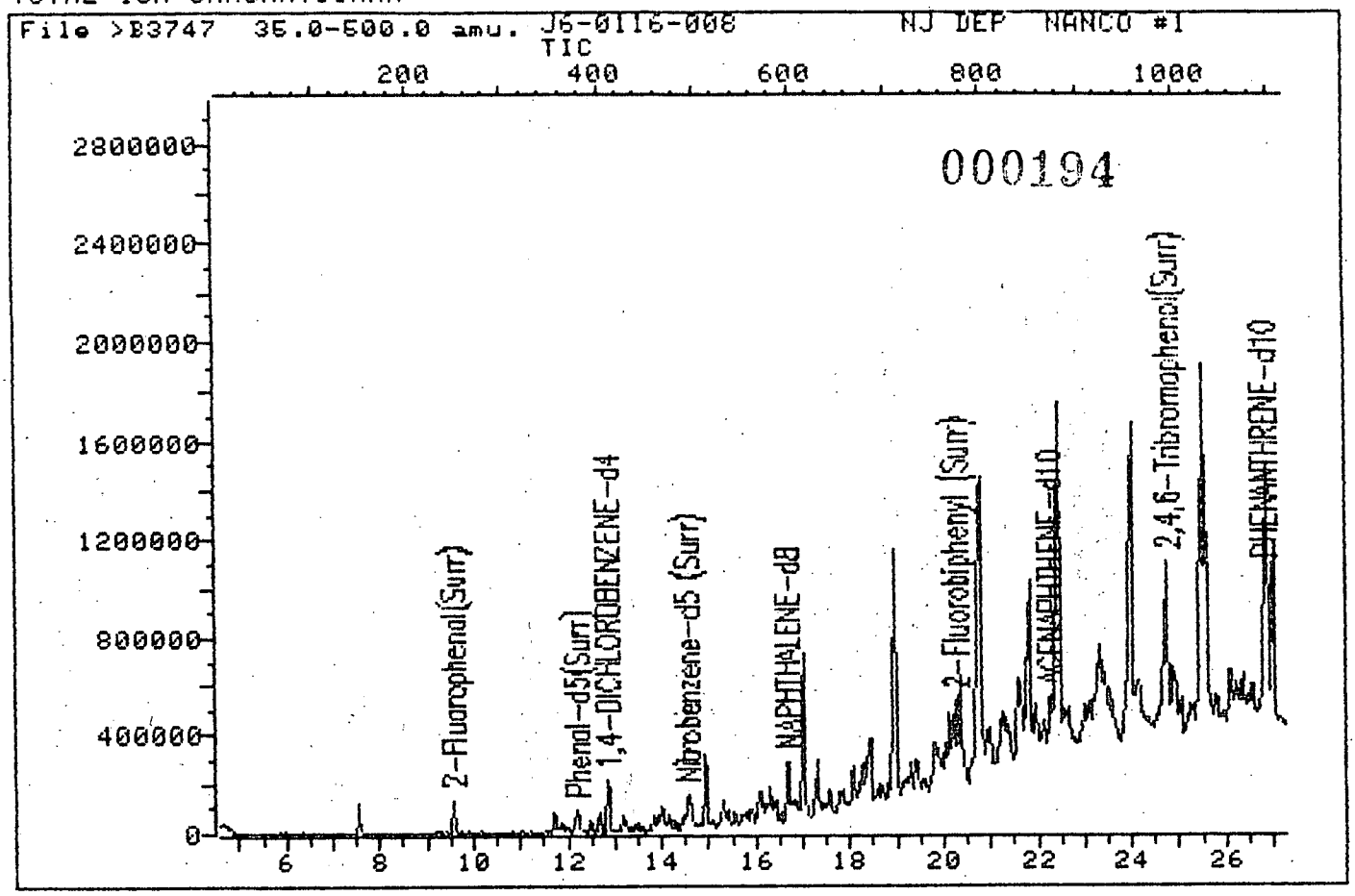
000193

	Compound	R.T.	Scan#	Area	Conc	Units	q
1)	*1,4-DICHLOROBENZENE-d4	12.85	407	109412	40.00	UG	97
14)	*NAPHTHALENE-d8	16.69	596	357809	40.00	UG	100
23)	Naphthalene	16.75	599	13186	~~109.10~~ (50)	UG 3.27	72
24)	4-Chloroaniline	17.04	613	17977	~~494.85~~	UG 14.82	85
27)	2-Methylnaphthalene	18.95	707	63645	~~795.37~~	UG 23.86	78
28)	*ACENAPHTHENE-d10	22.27	870	164872	40.00	UG	92
41)	2,4-Dinitrotoluene	23.03	907	11773	~~437.60~~	UG 13.13	90
45)	Fluorene	23.94	952	26519	~~335.51~~	UG 10.06	66
47)	*PHENANTHRENE-d10	26.83	1093	297338	40.00	UG	95
49)	N-Nitrosodiphenylamine	24.76	992	74585	~~1760.28~~	UG 52.81	65
53)	Phenanthrene	26.89	1096	58537	~~623.87~~	UG 18.72	97
57)	*CHRYSENE-d12	35.00	1493	222019	40.00	UG	100
62)	bis(2-Ethylhexyl)Phthalate	35.57	1521	260516	~~2550.63~~	UG 76.76	87
64)	*PERYLENE-d12	39.12	1695	92688	40.00	UG	100
65)	Di-n-Octyl Phthalate	37.37	1609	283959	~~2161.92~~	UG 64.86	100
72)	* 1,4 Dichlorobenzene(IS)	12.85	407	109412	40.00	UG	97
73)	Phenol-d5(Surr)	12.20	375	108447	~~2170.67~~	UG 65.36	85
74)	2-Fluorophenol(Surr)	9.57	245	112166	~~2404.23~~	UG 72.13	89
75)	*Naphthalene-d8 (IS)	16.69	596	357809	40.00	UG	93
76)	Nitrobenzene-d5 (Surr)	14.56	491	144890	~~2480.49~~	UG 74.42	91
77)	*Acenaphthene-d10 (IS)	22.27	870	164872	40.00	UG	92
78)	2-Fluorobiphenyl (Surr)	20.25	771	243647	~~2683.07~~	UG 80.49	98
79)	2,4,6-Tribromophenol(Surr)	24.76	992	72780	~~3865.76~~	UG 115.97	93
80)	*Chrysene-d12 (IS)	35.00	1493	222019	40.00	UG	100
81)	Terphenyl-d14 (Surr)	31.90	1341	273494	~~4060.10~~	UG 121.80	97

(50)

* Compound is ISTD

TOTAL ION CHROMATOGRAM



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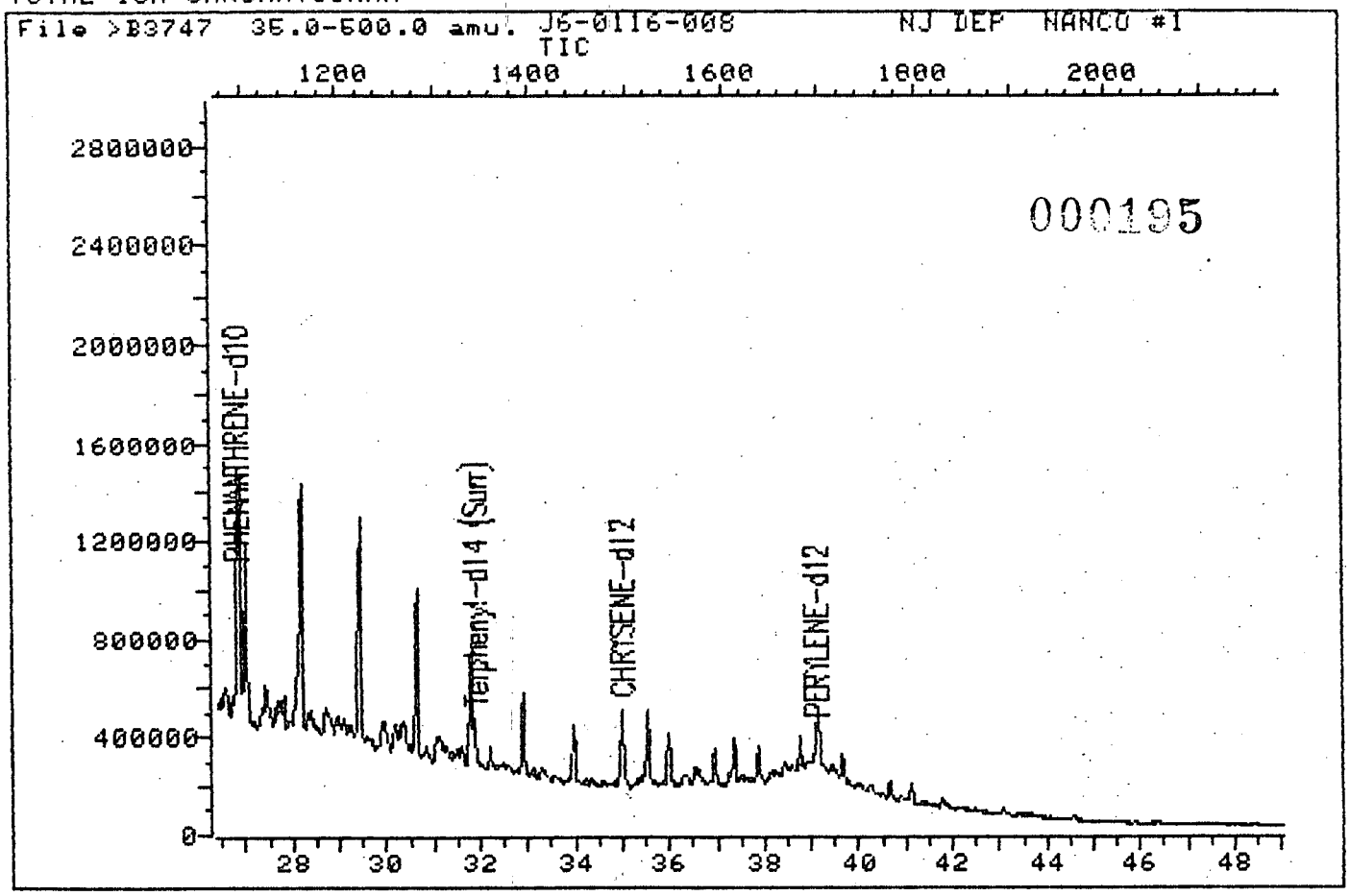
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3

Id File: IDEPA1::NA
Title: IDEPA BNA
Last Calibration: 861023 09:48

Operator ID: MORRIS
Quant Time: 861023 09:57
Injected at: 861022 18:13

TIC page 1 of 2

TOTAL ION CHROMATOGRAM



000195

Data File: >B3747::D1
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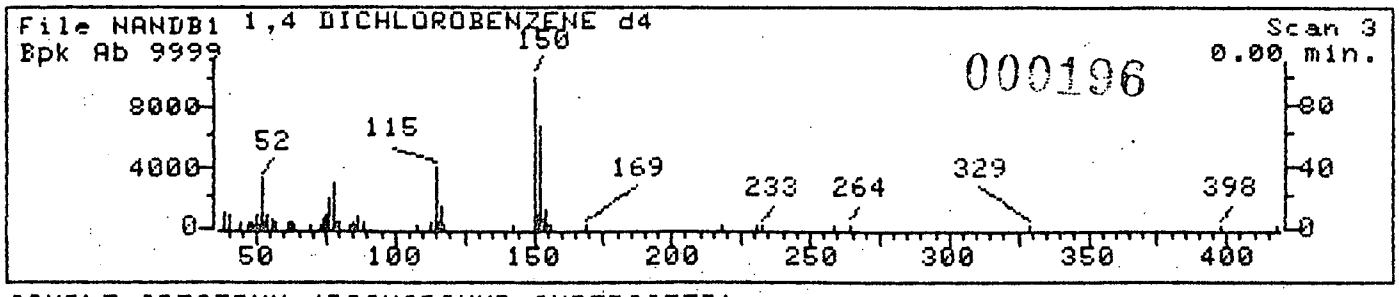
Misc: NJ DEP NANCO #1 BTL# 3

Id File: IDEPA1::NA
Title: IDEPA BNA
Last Calibration: 861023 09:48

Operator ID: MORRIS
Quant Time: 861023 09:57
Injected at: 861022 18:13

TIC page 2 of 2

REFERENCE STANDARD SPECTRUM



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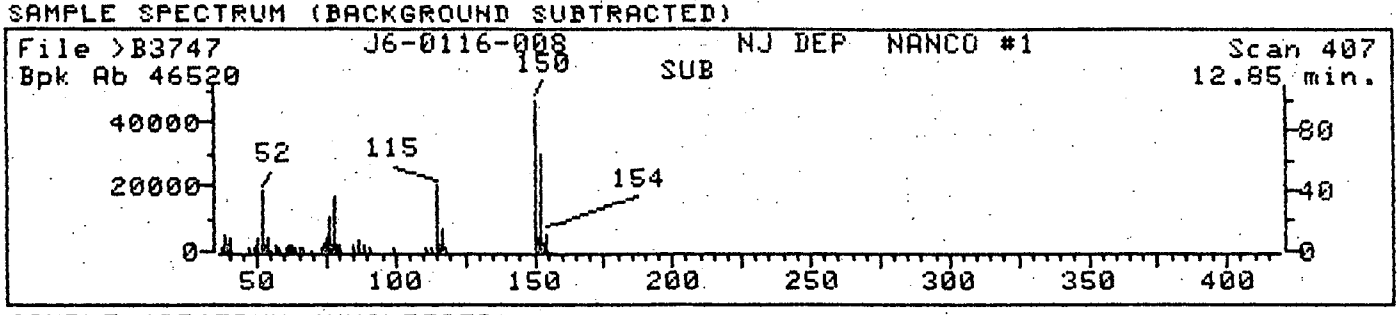

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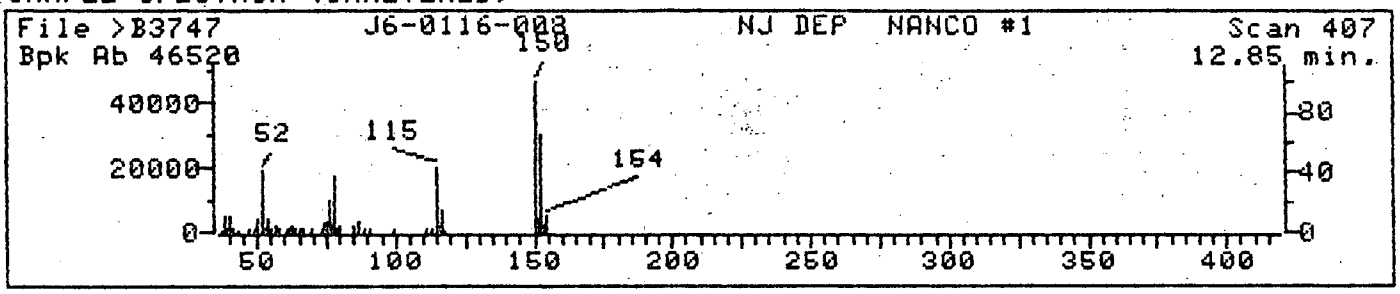
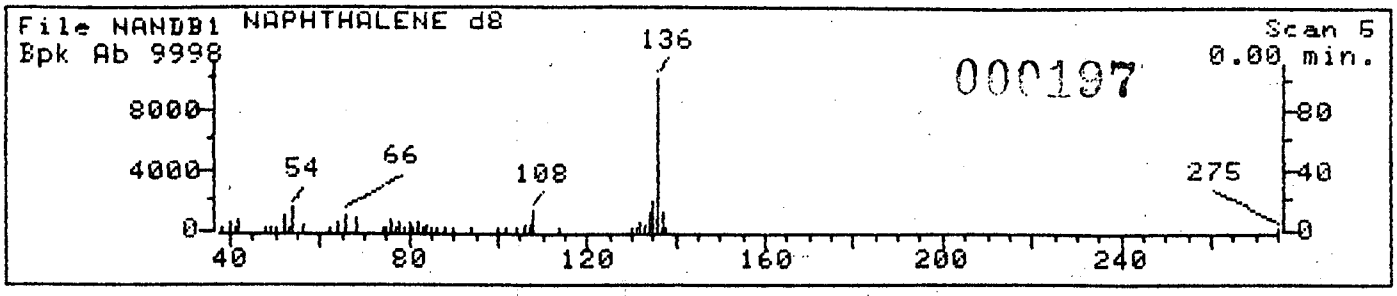


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 1 (ISTD)
Compound Name: 1,4-DICHLOROBENZENE-d4
Scan Number: 407
Retention Time: 12.85 min.
Area: 109412
Concentration: 40.00 UG
q-value: 97

REFERENCE STANDARD SPECTRUM



000197

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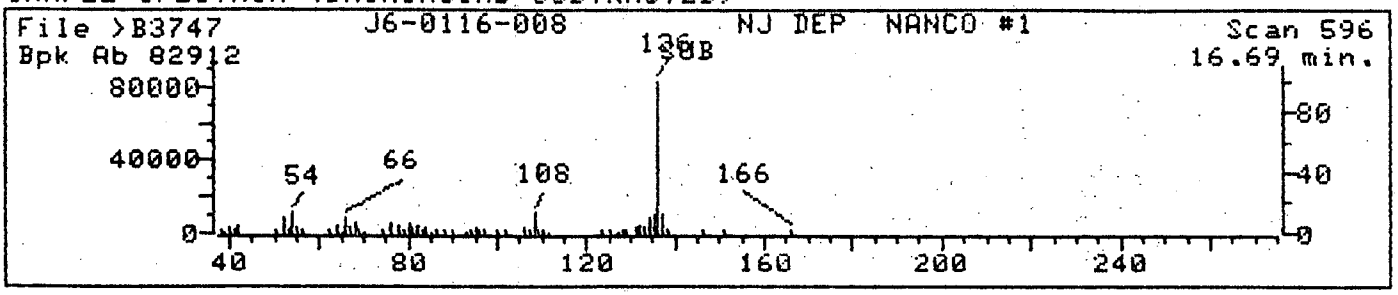

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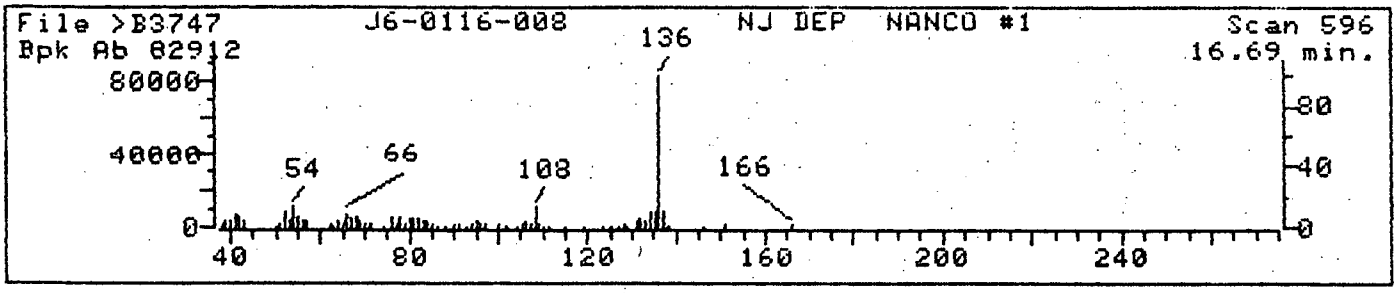
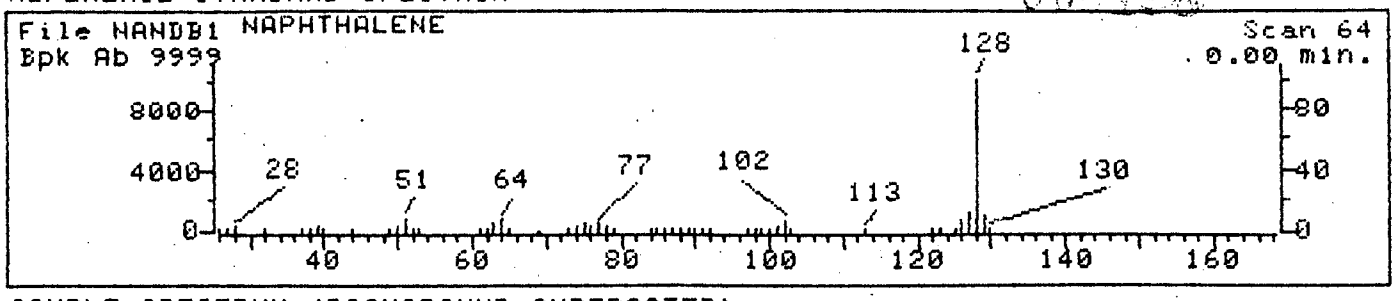


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 14 (ISTD)
Compound Name: NAPHTHALENE-d8
Scan Number: 596
Retention Time: 16.69 min.
Area: 357809
Concentration: 40.00 UG
q-value: 100

REFERENCE STANDARD SPECTRUM



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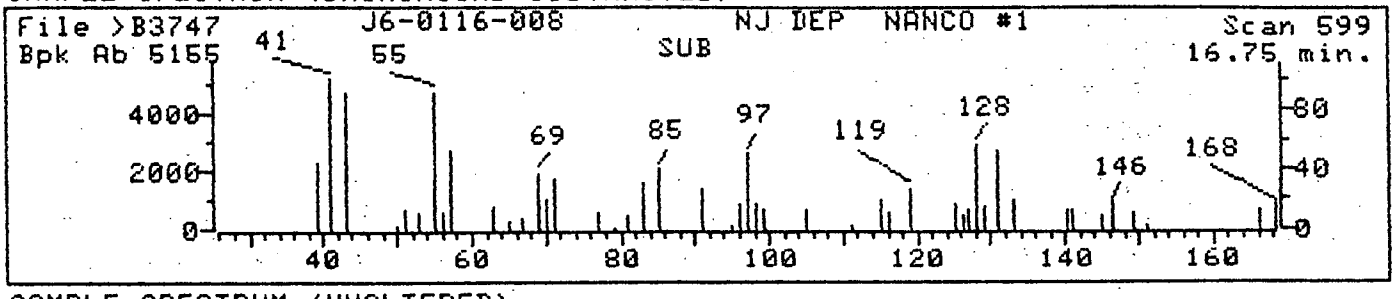

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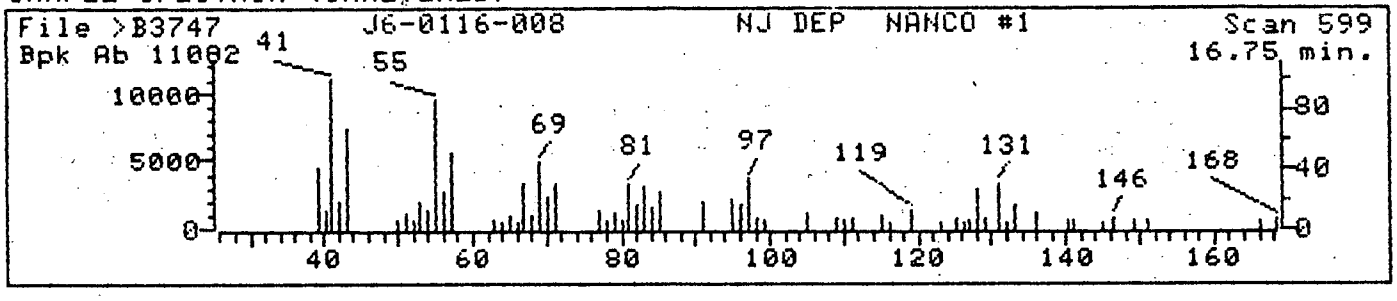

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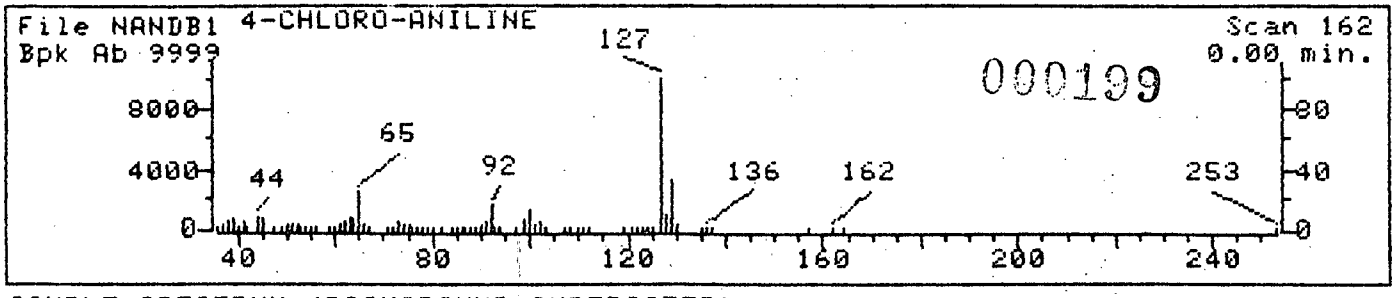
Name: J6-0116-008
Misc: NJ DEP NANCO #1
Quant Time: 861023 09:57
Injected at: 861022 18:13

BTL# 3

Compound No: 23
Compound Name: Naphthalene
Scan Number: 599
Retention Time: 16.75 min.
Area: 13186
Concentration: ~~109.10 UG~~ 3.27
q-value: 72

REFERENCE STANDARD SPECTRUM



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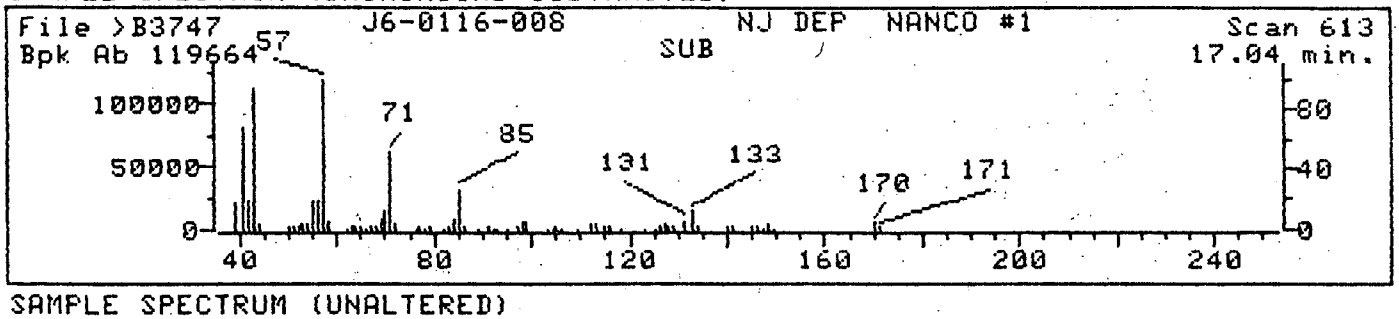

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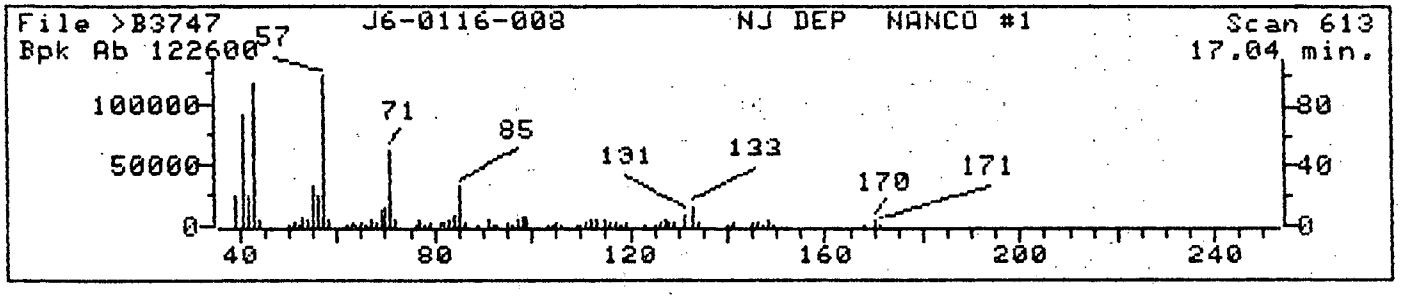
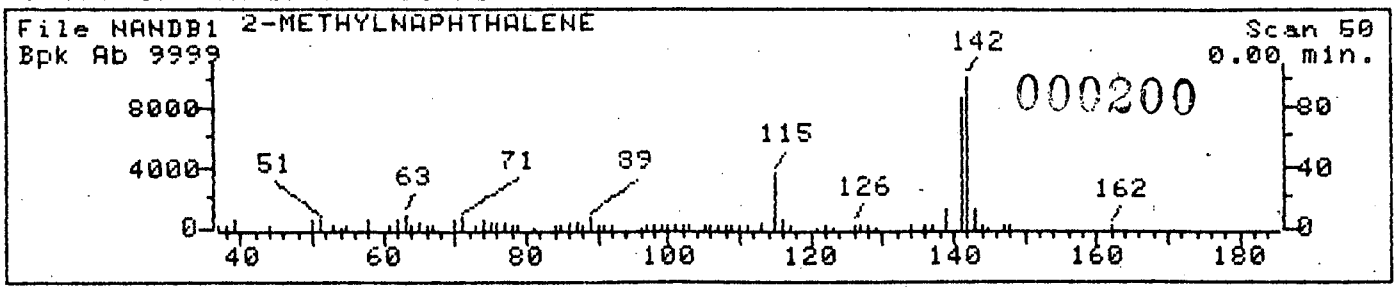


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 24
Compound Name: 4-Chloroaniline
Scan Number: 613
Retention Time: 17.04 min.
Area: 17977
Concentration: ~~494.05~~ UG
q-value: 85 94.82

✓ 26

REFERENCE STANDARD SPECTRUM



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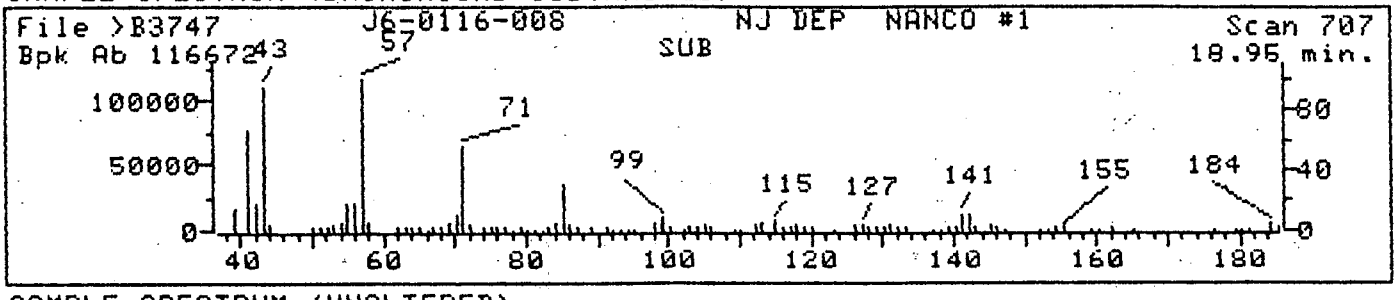

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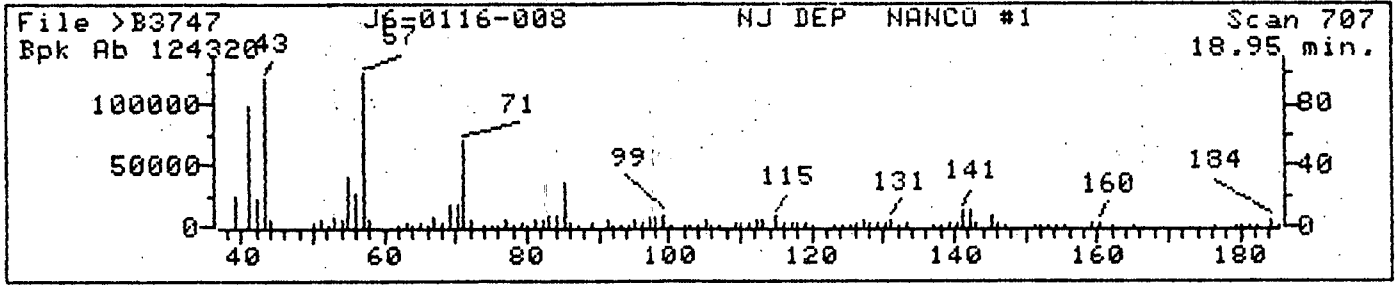
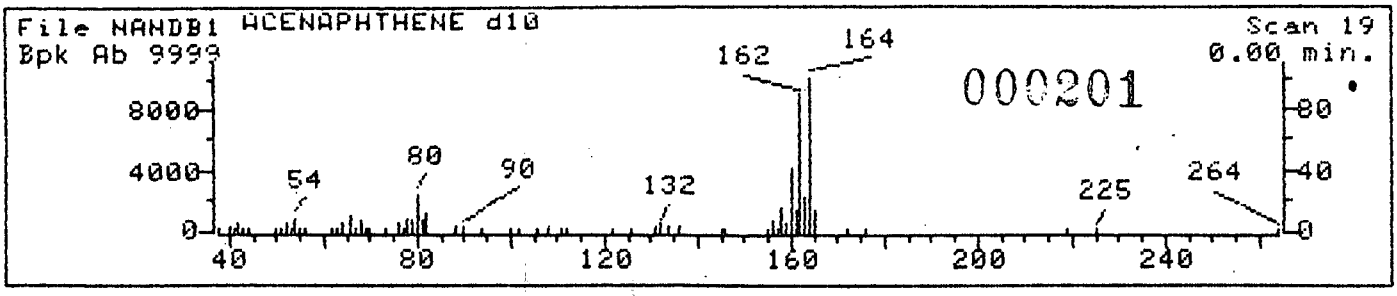


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 27
Compound Name: 2-Methylnaphthalene
Scan Number: 707
Retention Time: 18.95 min.
Area: 63645
Concentration: ~~795.37~~ UG
23.86
q-value: 78

V 56

REFERENCE STANDARD SPECTRUM



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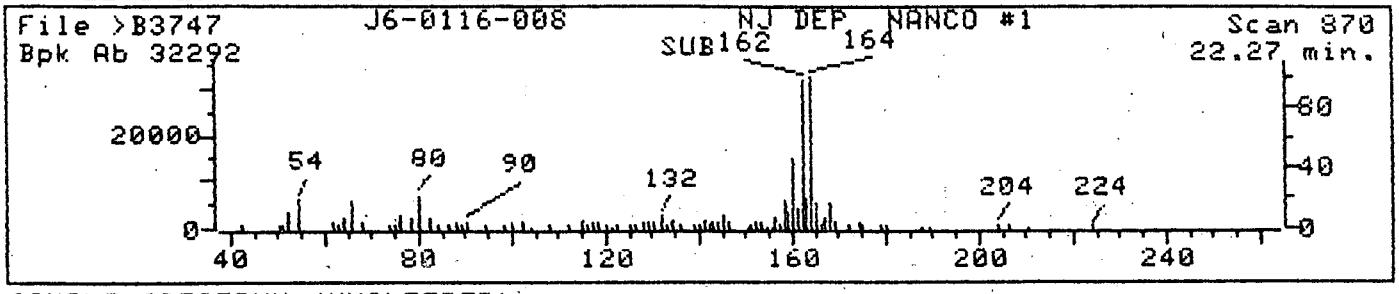

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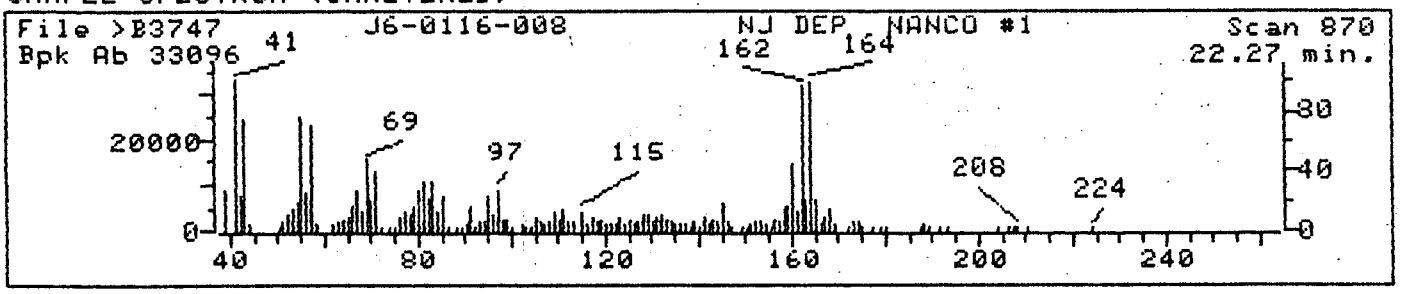
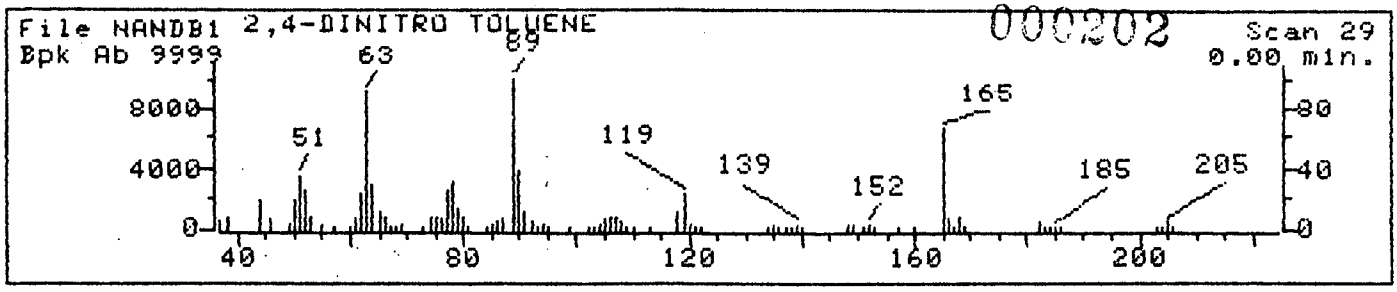


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 28 (ISTD)
Compound Name: ACENAPHTHENE-d10
Scan Number: 870
Retention Time: 22.27 min.
Area: 164872
Concentration: 40.00 UG
q-value: 92

REFERENCE STANDARD SPECTRUM



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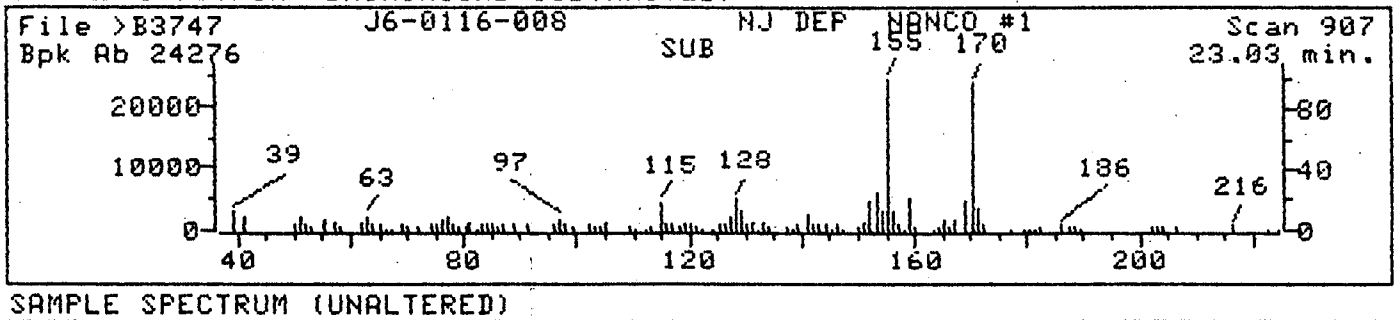

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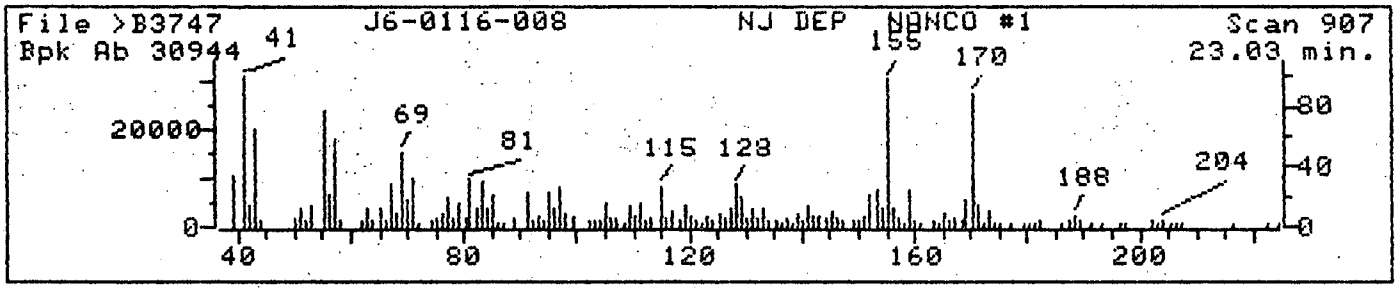


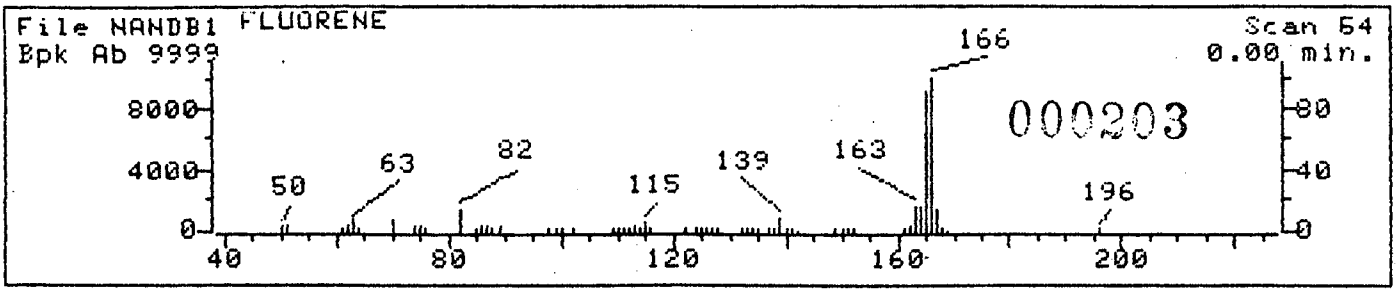
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 41
Compound Name: 2,4-Dinitrotoluene
Scan Number: 907
Retention Time: 23.03 min.
Area: 11773
Concentration: ~~437.60~~ UG
q-value: 90

13.13

VSG

REFERENCE STANDARD SPECTRUM



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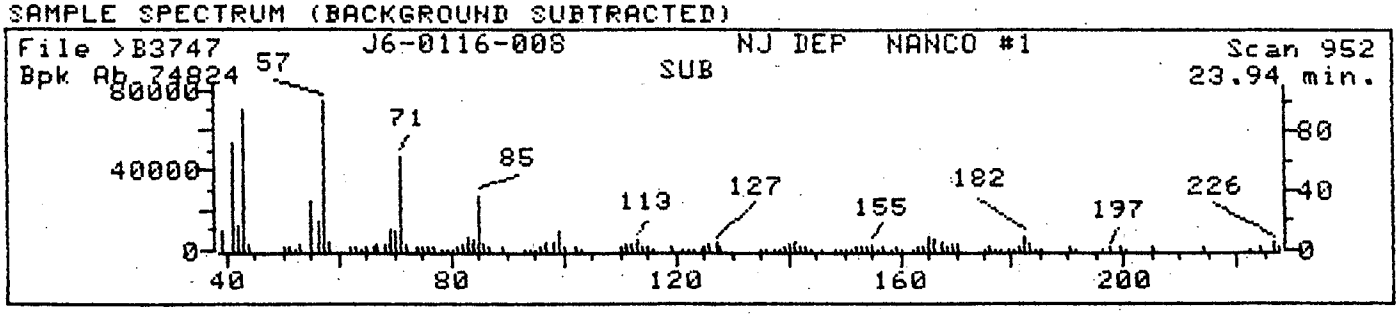

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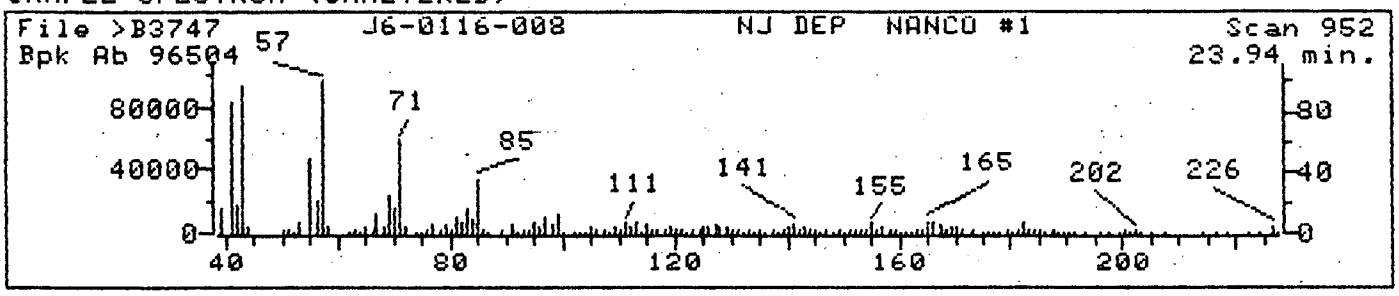
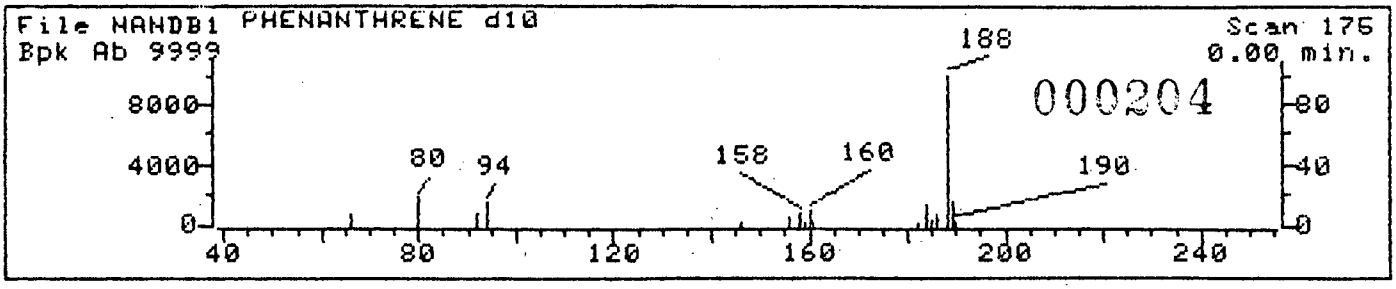


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 45
Compound Name: Fluorene
Scan Number: 952
Retention Time: 23.94 min.
Area: 26519
Concentration: ~~335.51~~ UG
q-value: 66 10.06

✓ 56

REFERENCE STANDARD SPECTRUM



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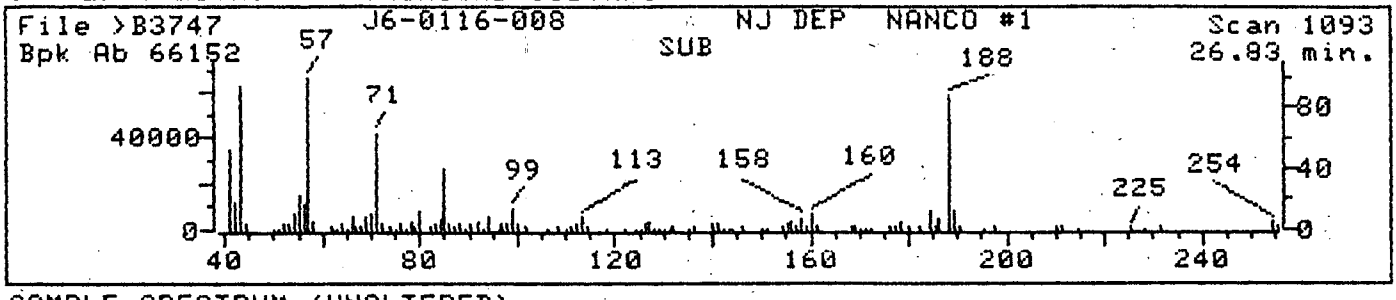

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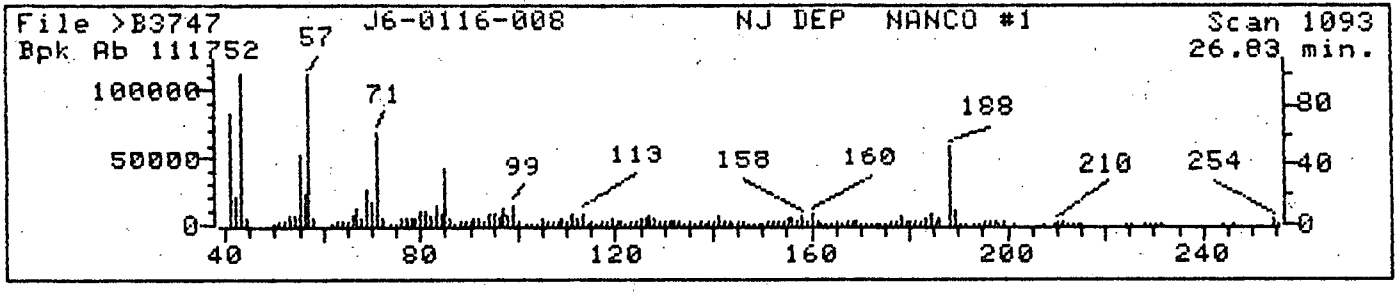
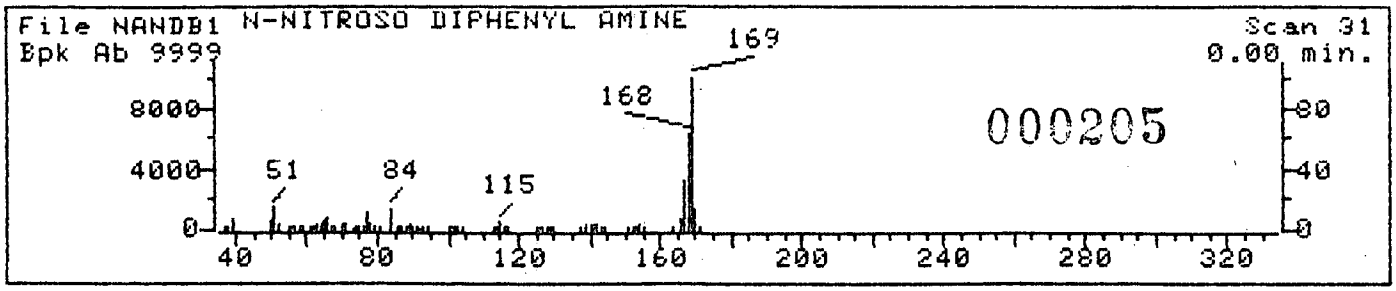


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 47 (ISTD)
Compound Name: PHENANTHRENE-d10
Scan Number: 1093
Retention Time: 26.83 min.
Area: 297338
Concentration: 40.00 UG
q-value: 95

REFERENCE STANDARD SPECTRUM



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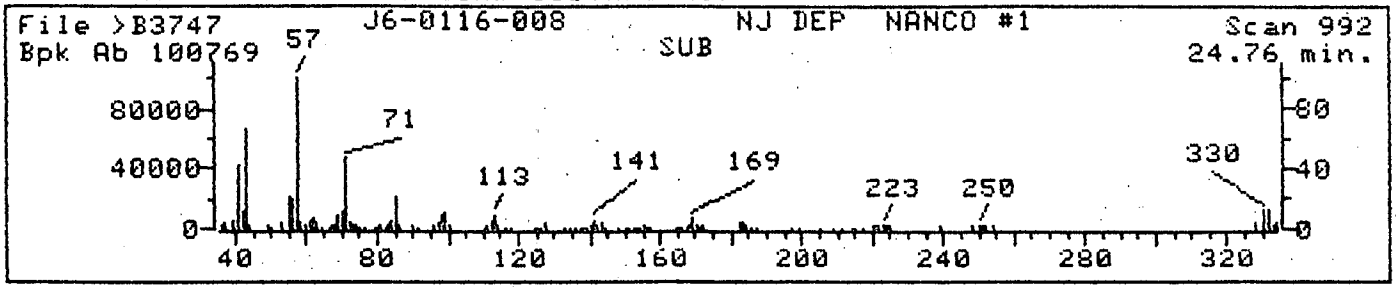

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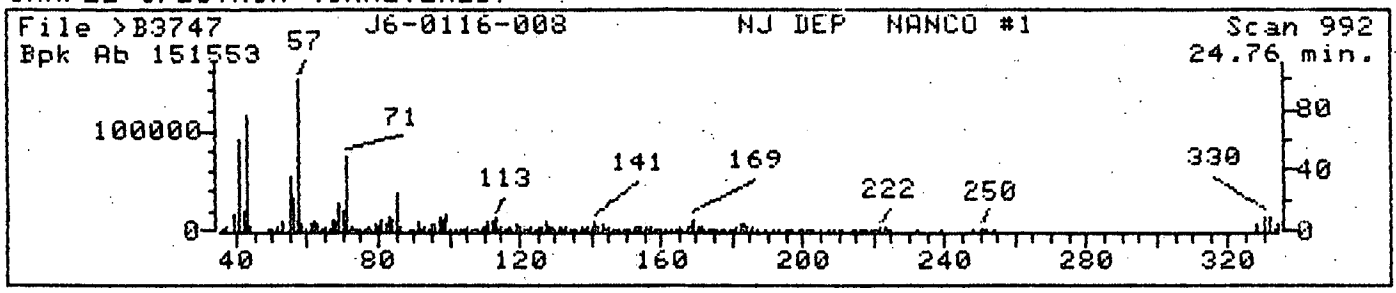
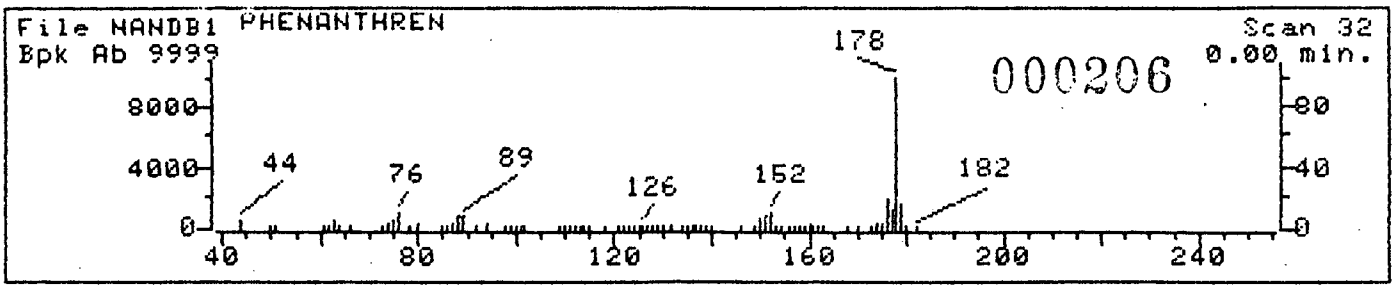


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 49
Compound Name: N-Nitrosodiphenylamine
Scan Number: 992
Retention Time: 24.76 min.
Area: 74585
Concentration: ~~1760.28~~ UG
q-value: 65 52.81

V46

REFERENCE STANDARD SPECTRUM



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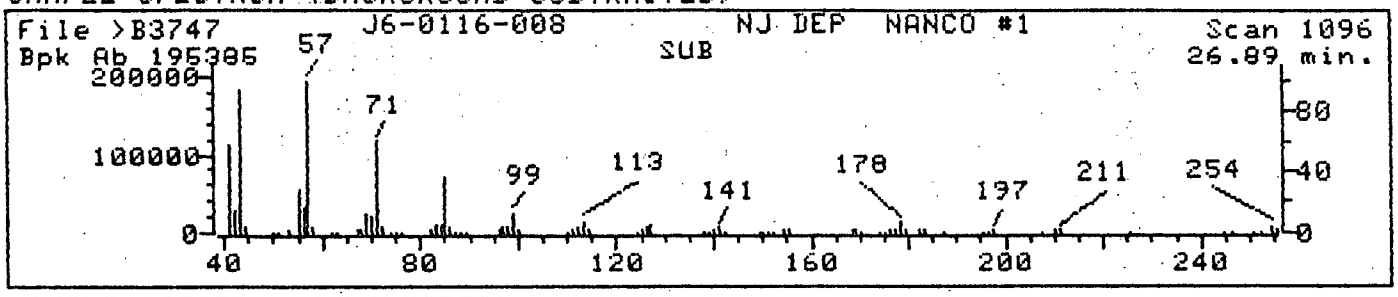

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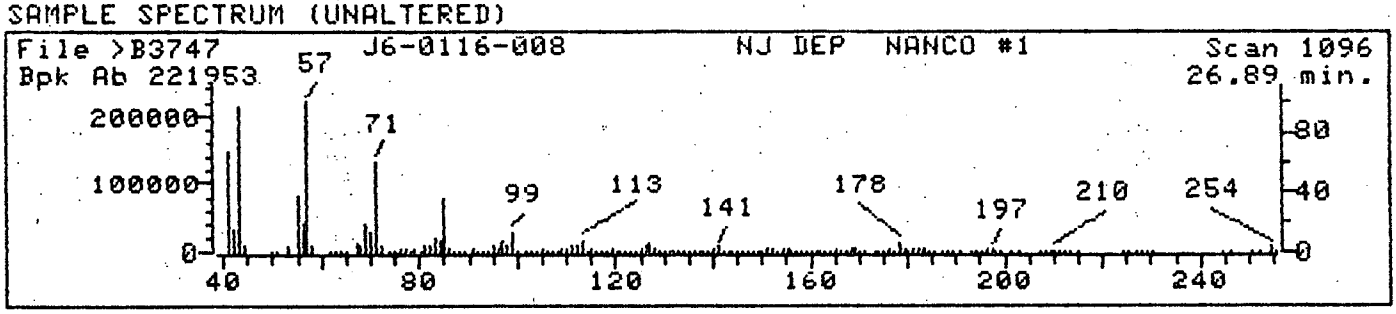


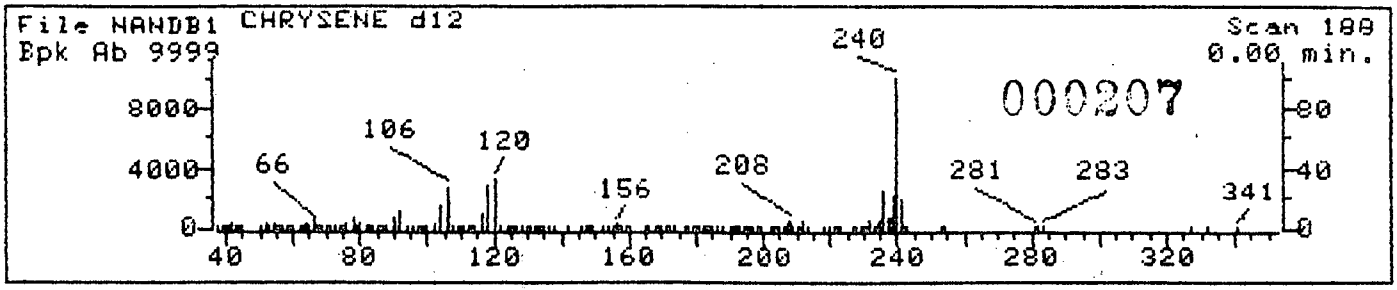
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 53
Compound Name: Phenanthrene
Scan Number: 1096
Retention Time: 26.89 min.
Area: 58537
Concentration: ~~823.87~~ UG
q-value: 97

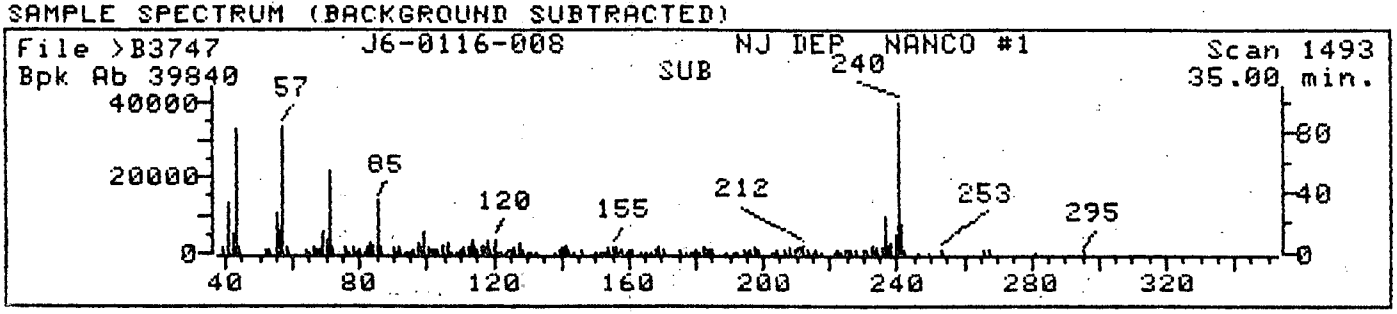
18.72

√ 50

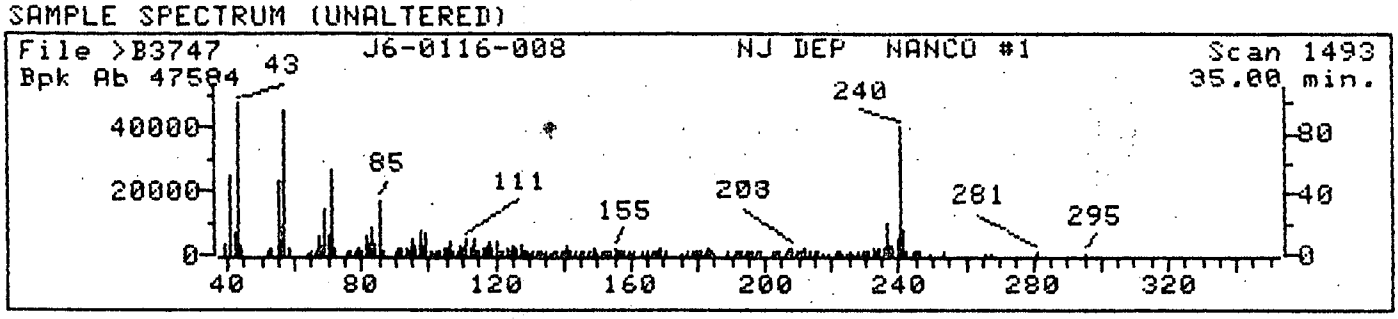
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



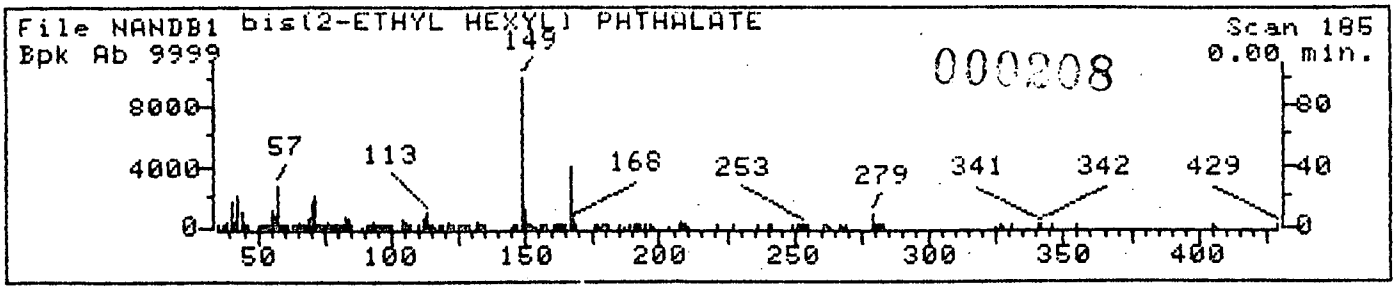
SAMPLE SPECTRUM (UNALTERED)



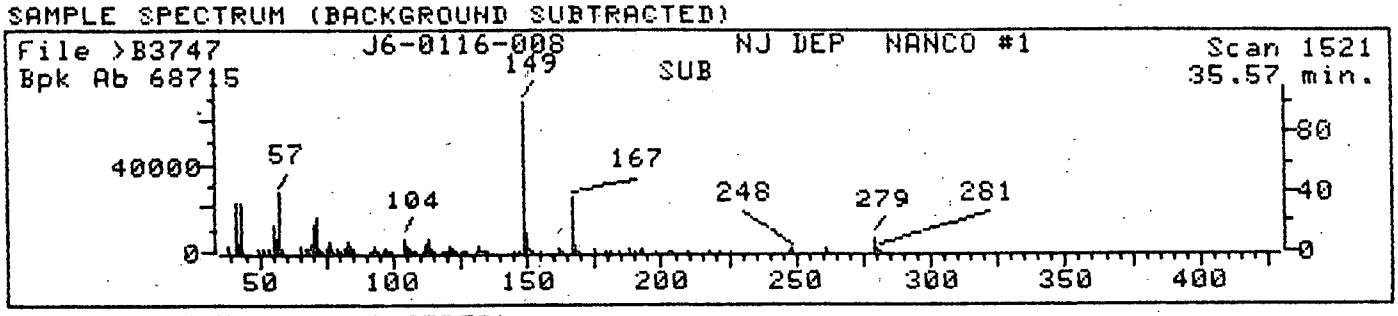
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 57 (ISTD)
Compound Name: CHRYSENE-d12
Scan Number: 1493
Retention Time: 35.00 min.
Area: 222019
Concentration: 40.00 UG
q-value: 100

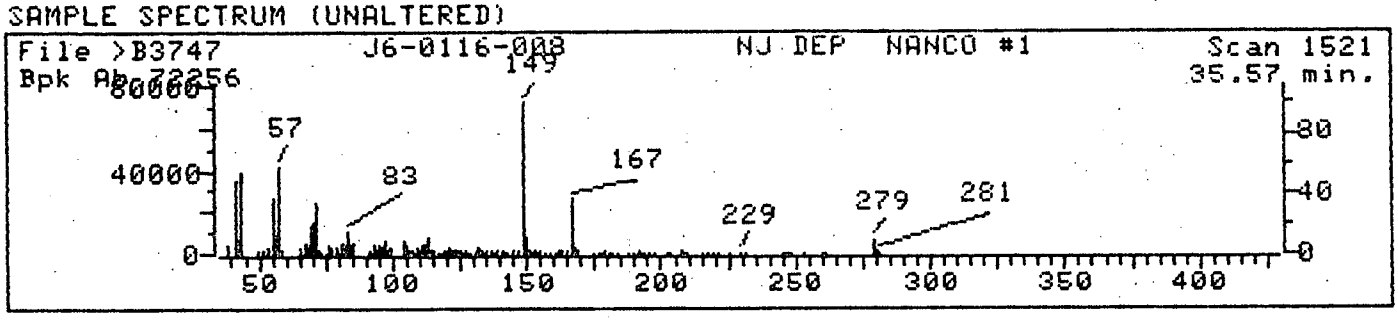
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



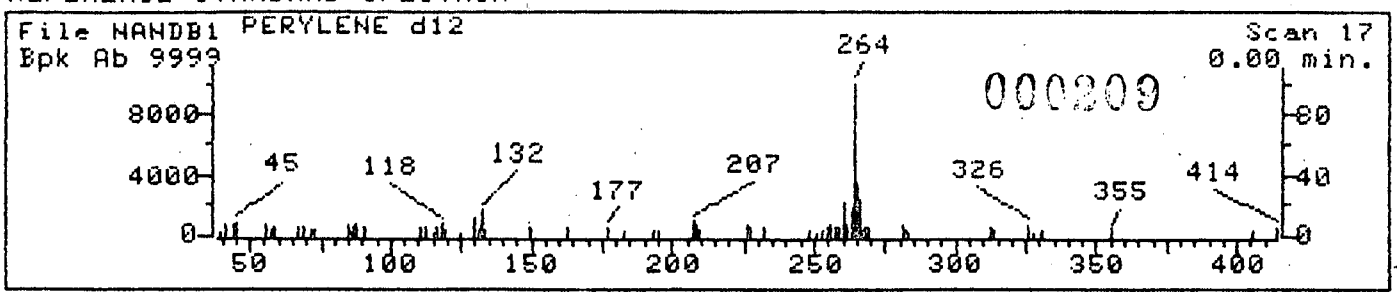
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 62
Compound Name: bis(2-Ethylhexyl)Phthalate
Scan Number: 1521
Retention Time: 35.57 min.
Area: 260516
Concentration: ~~2558.63~~ UG
q-value: 87

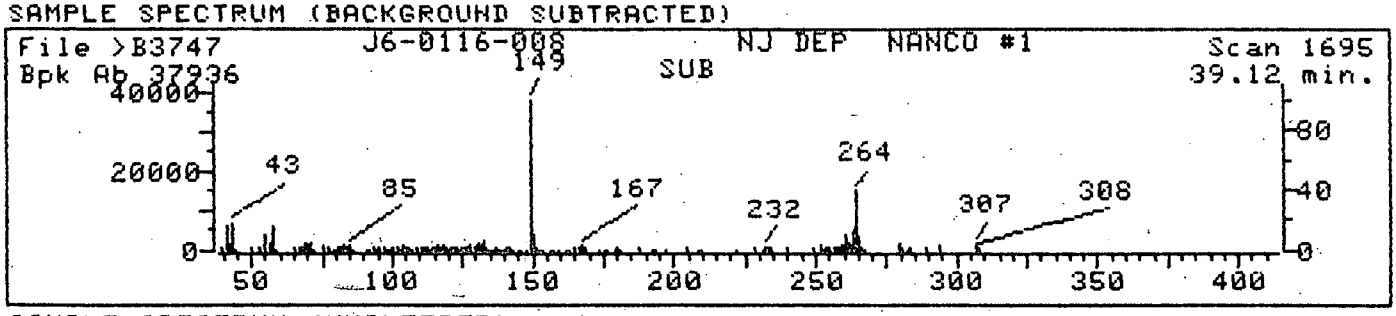
76.76

V 50

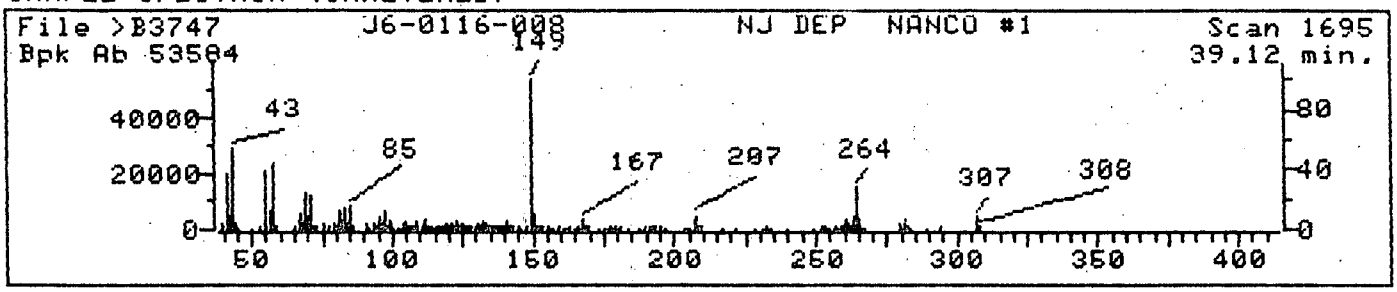
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



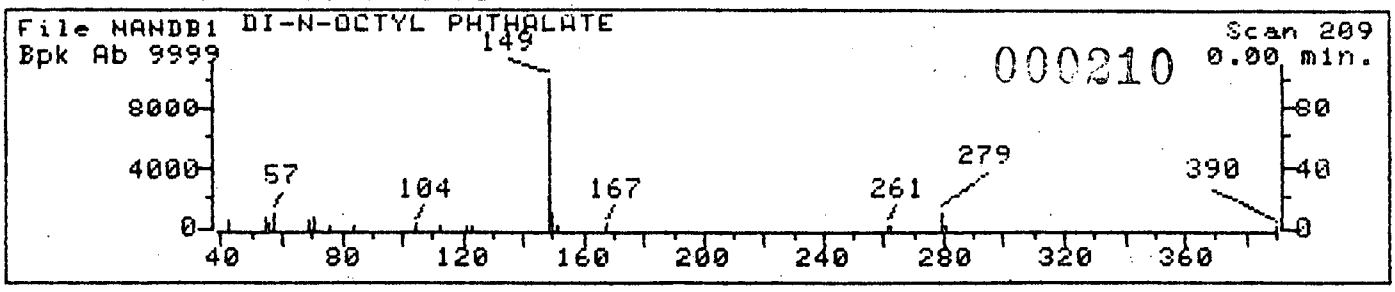
SAMPLE SPECTRUM (UNALTERED)



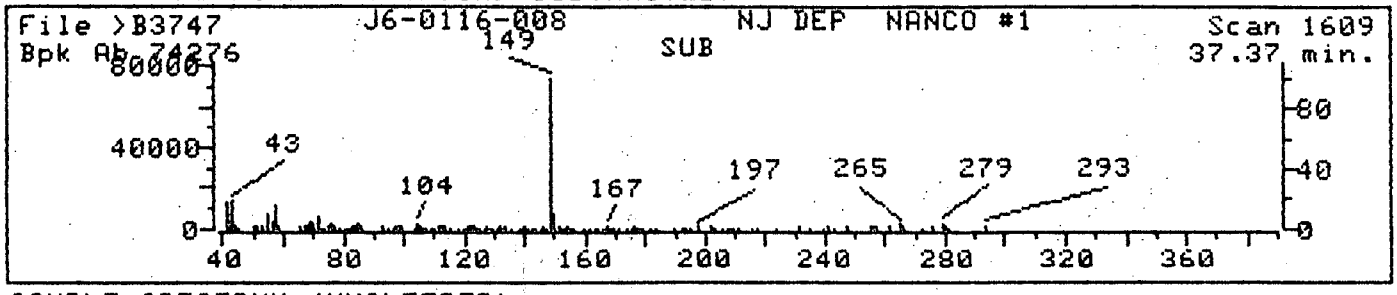
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 64 (ISTD)
Compound Name: PERYLENE-d12
Scan Number: 1695
Retention Time: 39.12 min.
Area: 92688
Concentration: 40.00 UG
q-value: 100

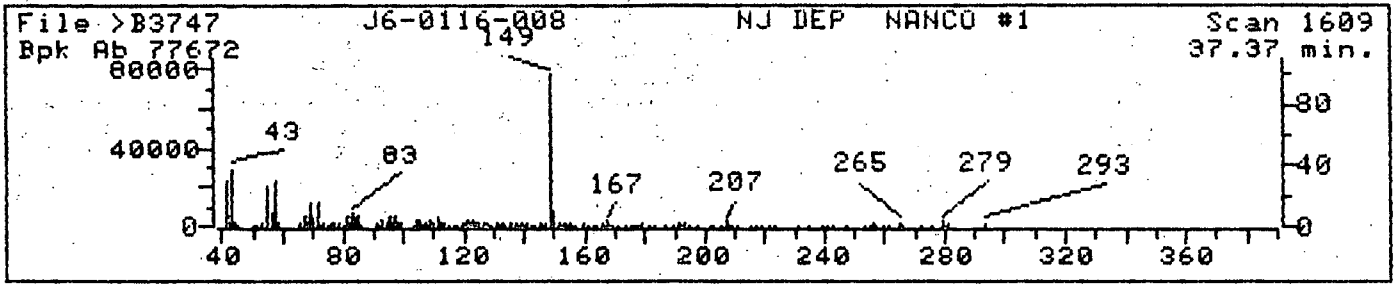
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



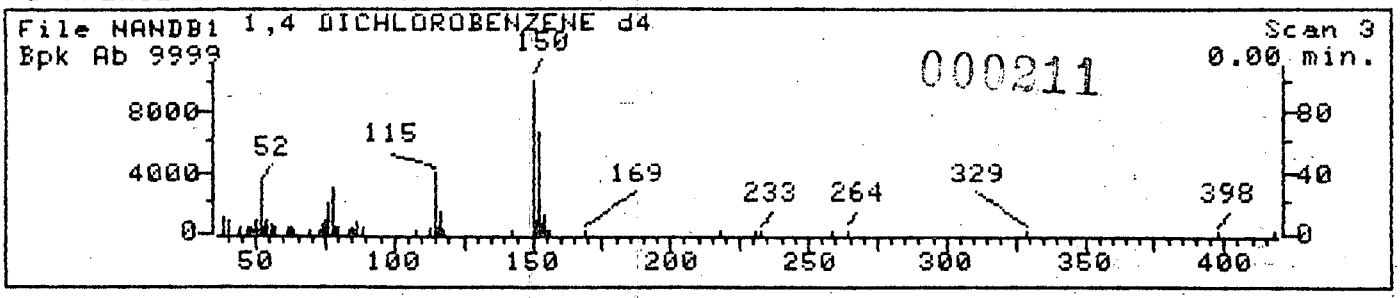
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 65
Compound Name: Di-n-Octyl Phthalate
Scan Number: 1609
Retention Time: 37.37 min.
Area: 283959
Concentration: ~~2161.92~~ UG
q-value: 100

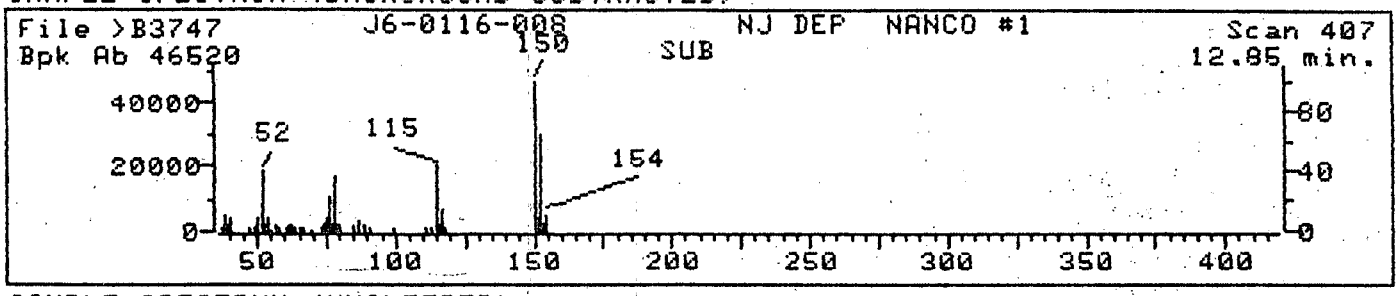
64.86

✓ 5

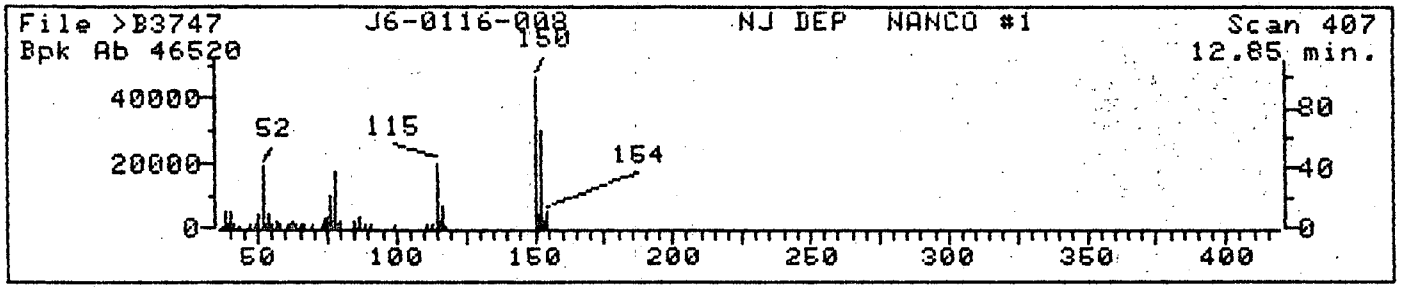
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



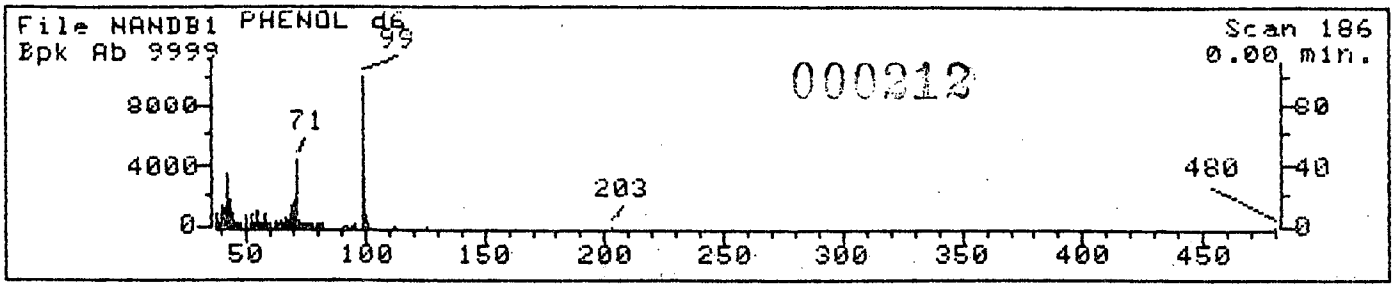
SAMPLE SPECTRUM (UNALTERED)



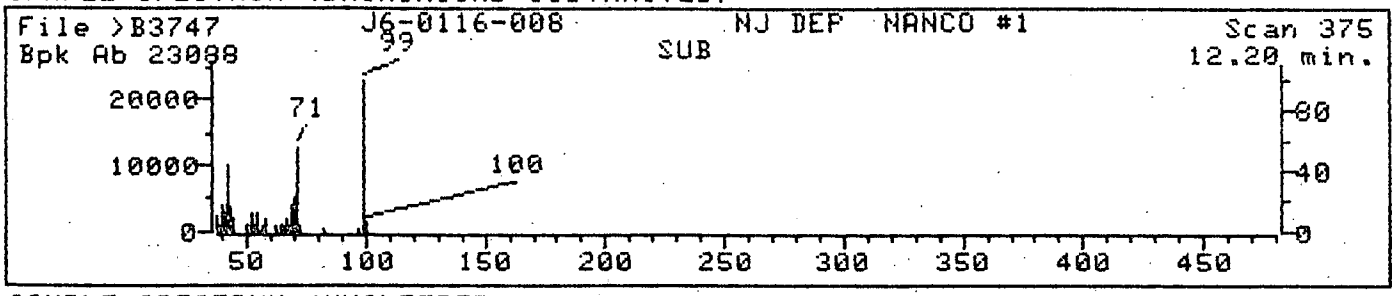
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 72 (ISTD)
Compound Name: 1,4 Dichlorobenzene(IS)
Scan Number: 407
Retention Time: 12.85 min.
Area: 109412
Concentration: 40.00 UG
q-value: 97

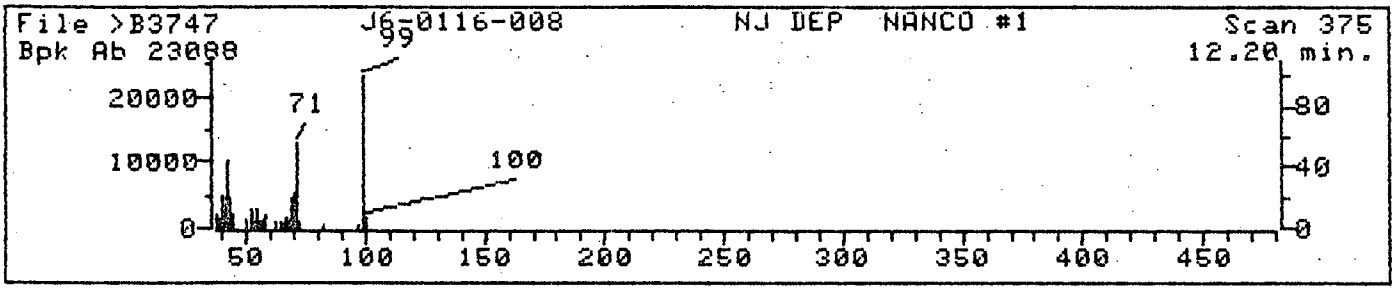
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)

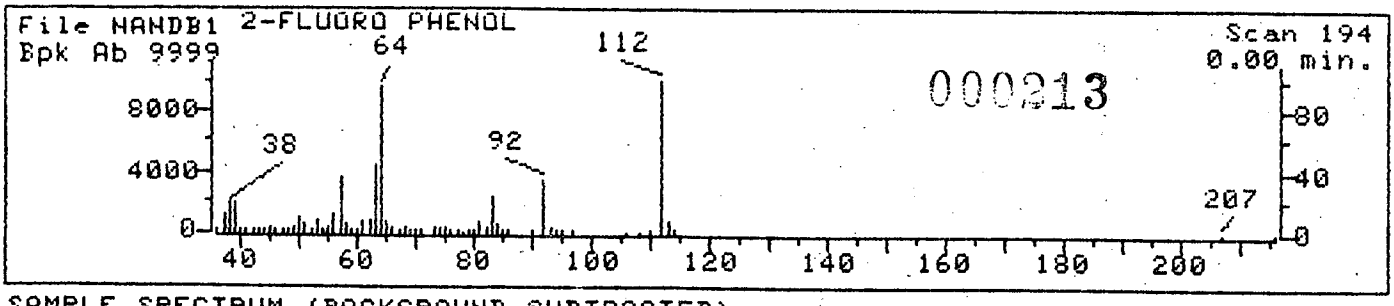


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

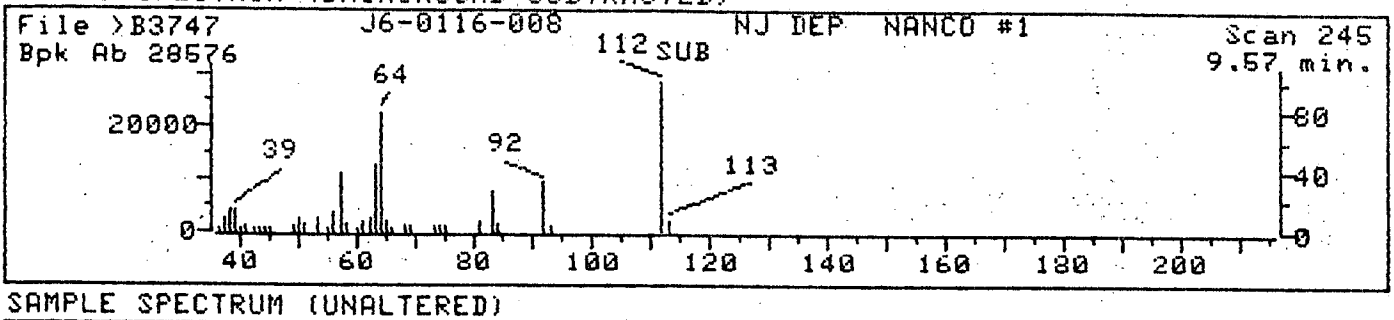
Compound No: 73
Compound Name: Phenol-d5(Surr)
Scan Number: 375
Retention Time: 12.20 min.
Area: 108447
Concentration: ~~2178.67~~ UG
q-value: 85

65.34

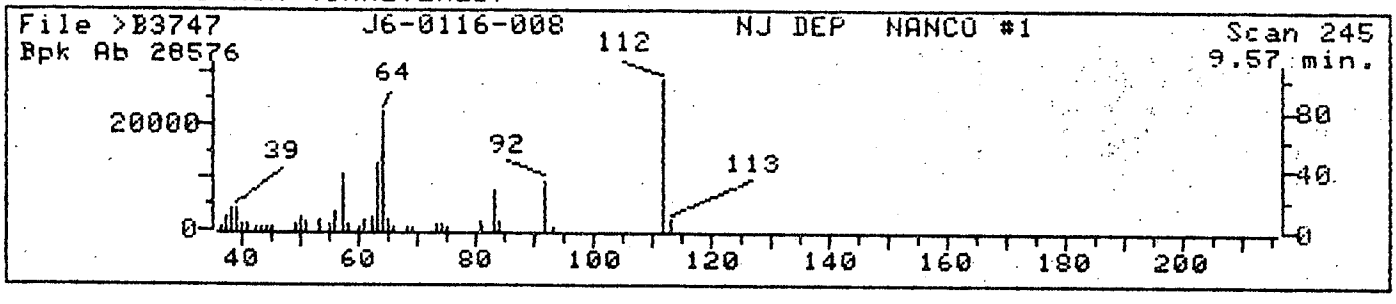
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)

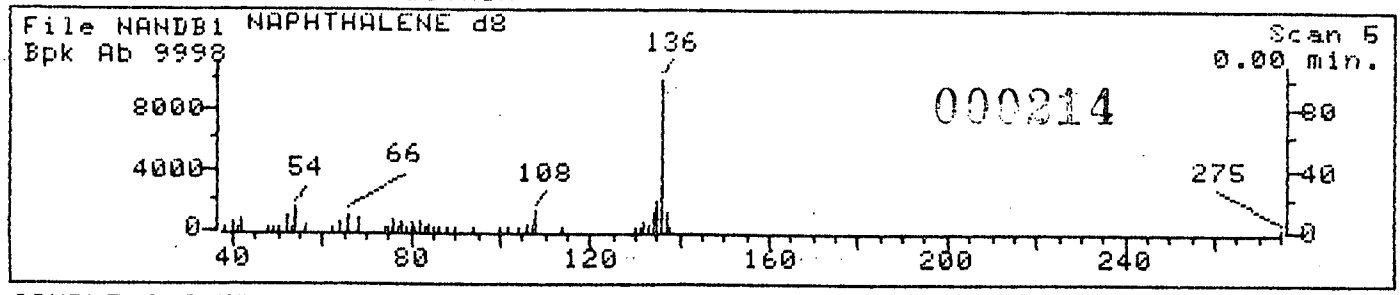


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 74
Compound Name: 2-Fluorophenol(Surr)
Scan Number: 245
Retention Time: 9.57 min.
Area: 112166
Concentration: ~~2404.23~~ UG
q-value: 89

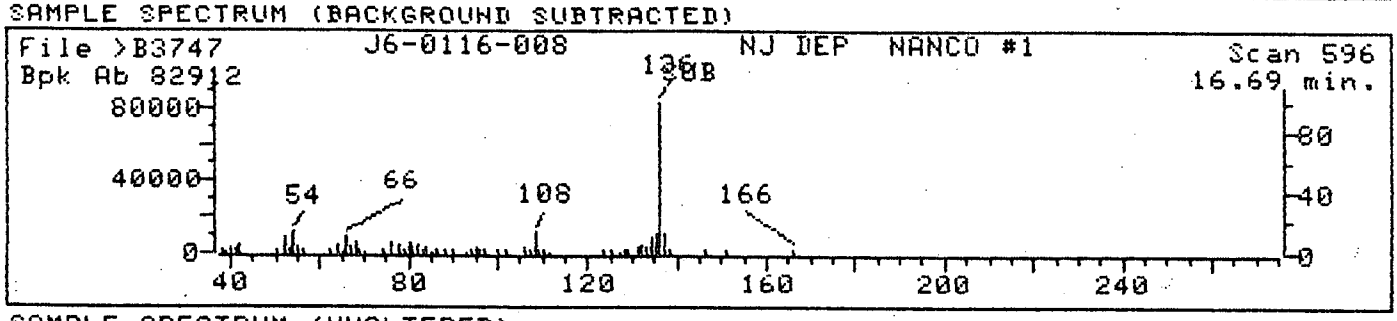
72.13

REFERENCE STANDARD SPECTRUM

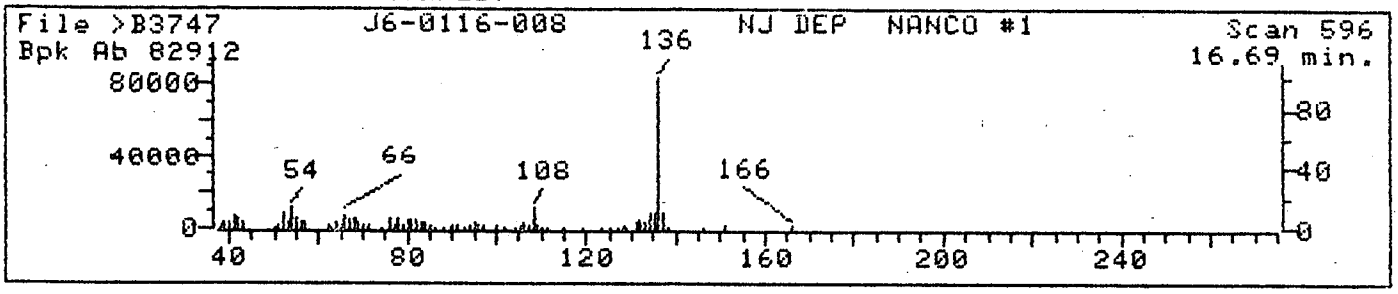


000214

SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



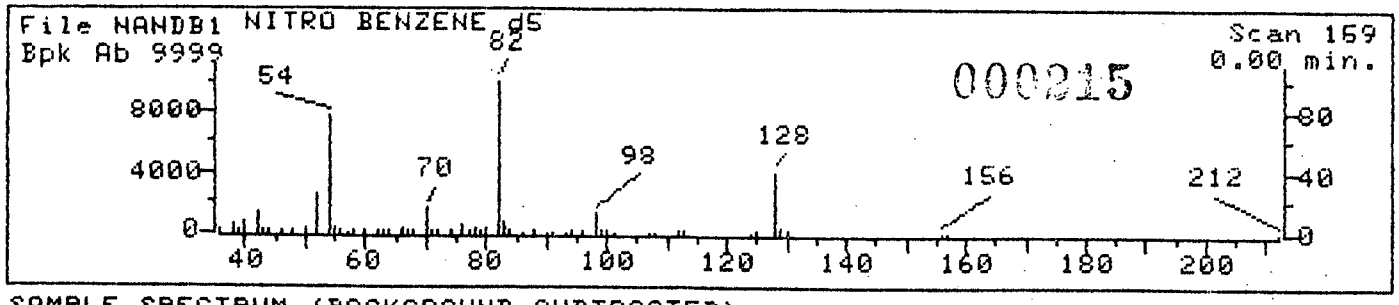
SAMPLE SPECTRUM (UNALTERED)



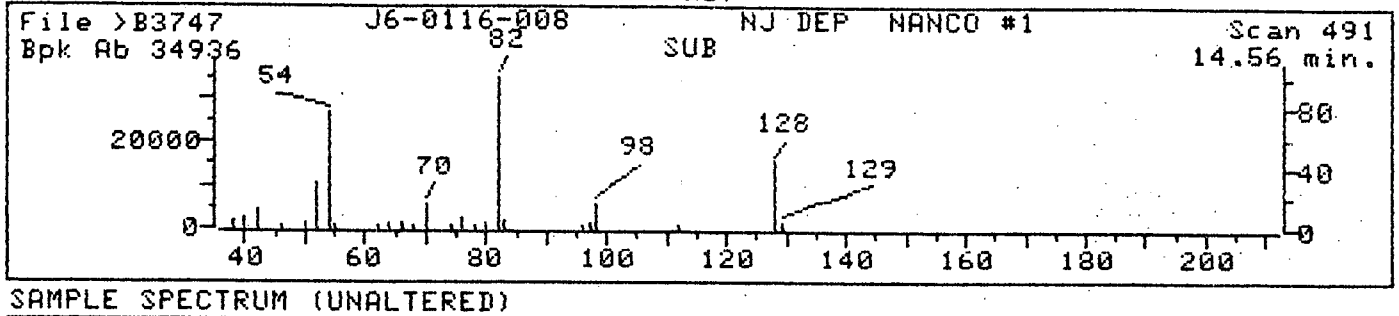
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 75 (ISTD)
Compound Name: Naphthalene-d8 (IS)
Scan Number: 596
Retention Time: 16.69 min.
Area: 357809
Concentration: 40.00 UG
q-value: 93

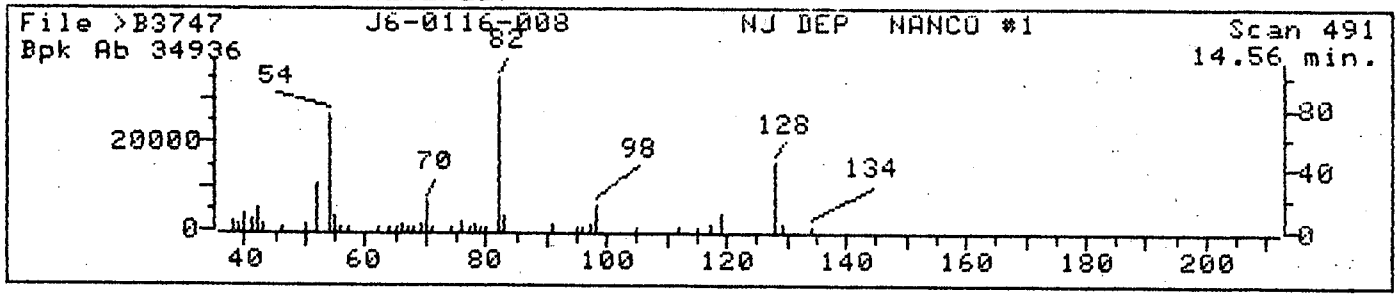
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)

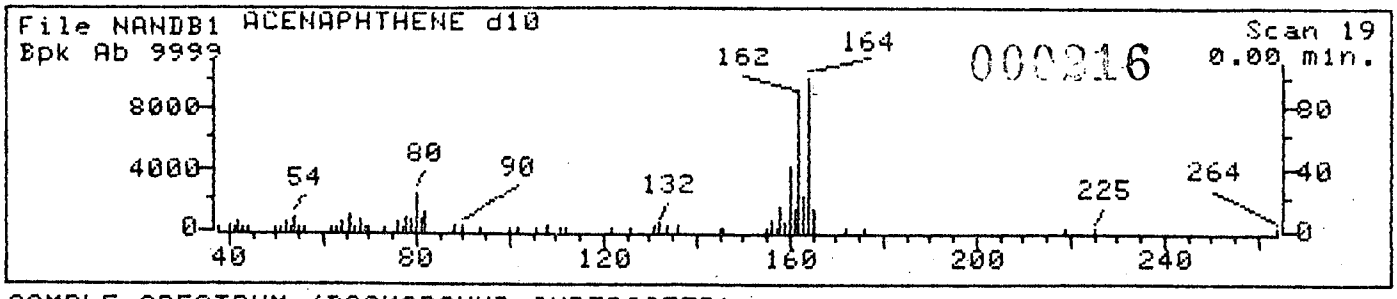


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

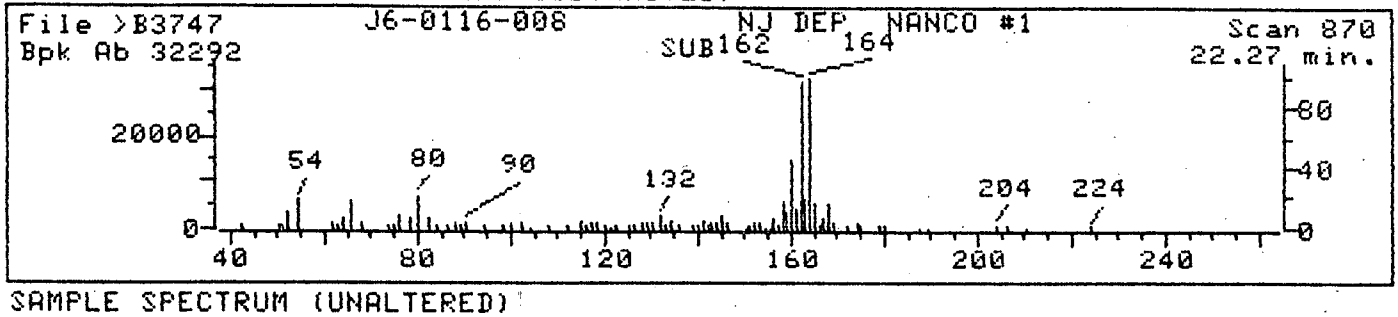
Compound No: 76
Compound Name: Nitrobenzene-d5 (Surr)
Scan Number: 491
Retention Time: 14.56 min.
Area: 144890
Concentration: ~~2480.49 UG~~ 74.42
q-value: 91

✓ 56

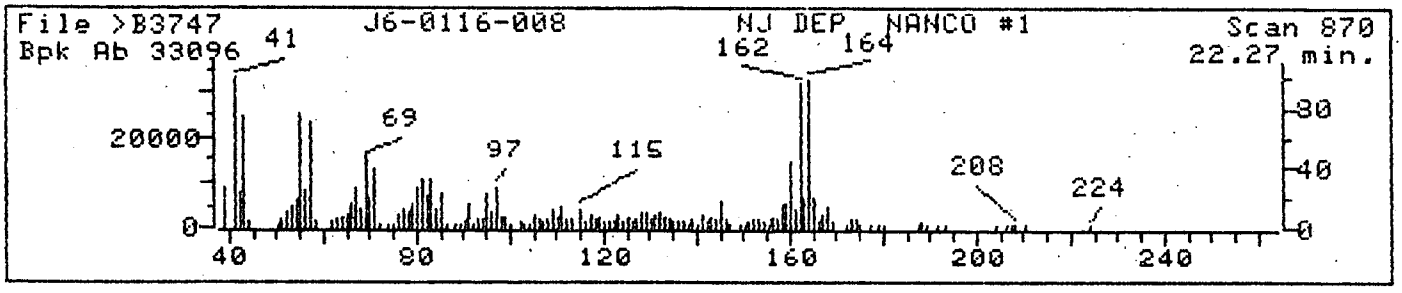
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



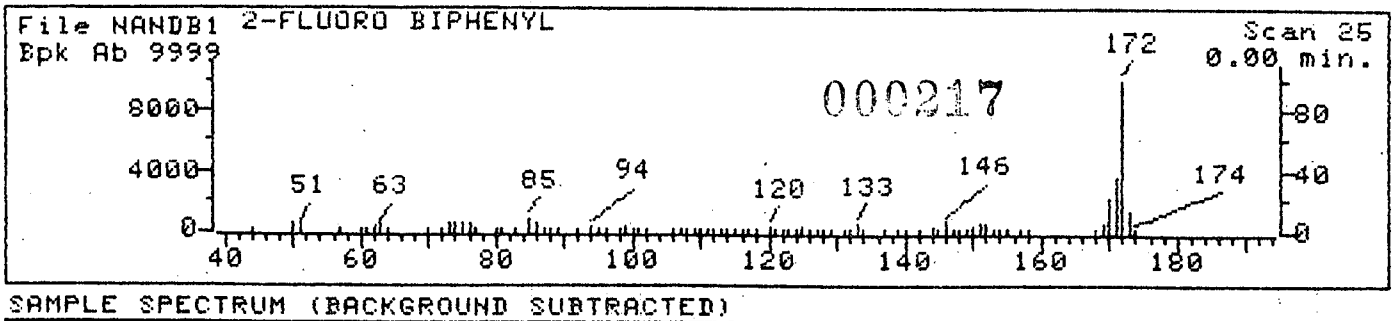
SAMPLE SPECTRUM (UNALTERED)



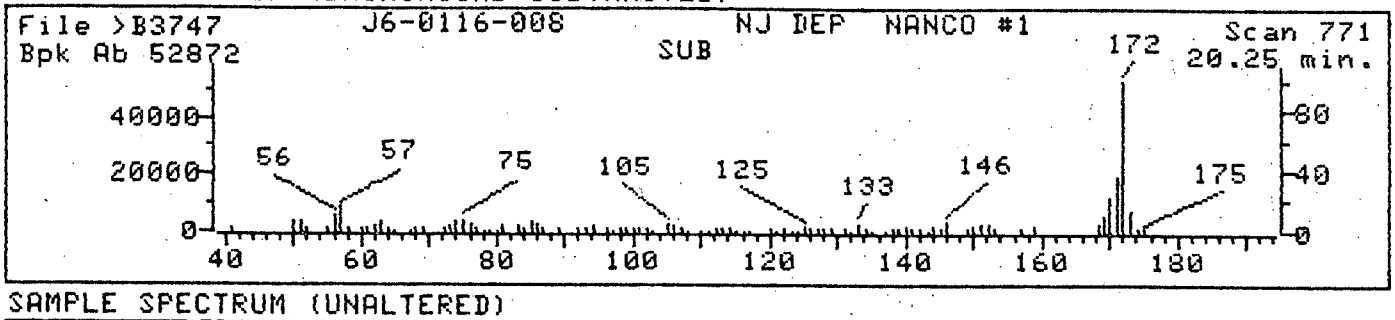
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 77 (ISTD)
Compound Name: Acenaphthene-d10 (IS)
Scan Number: 870
Retention Time: 22.27 min.
Area: 164872
Concentration: 40.00 UG
q-value: 92

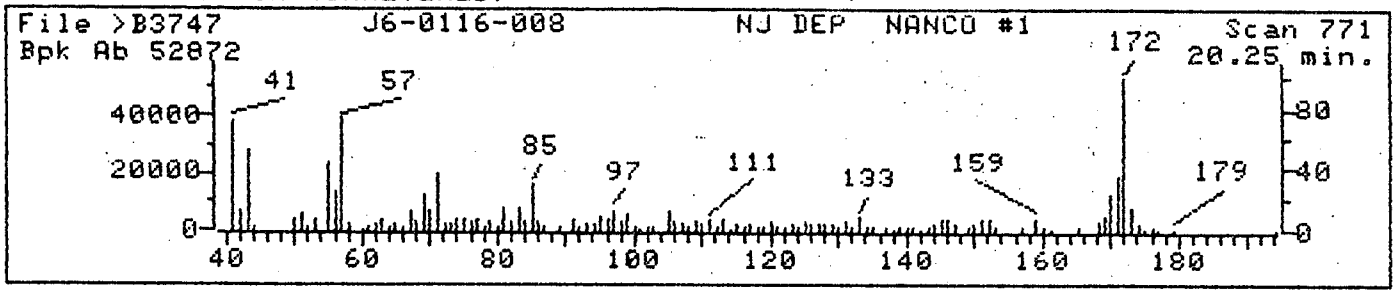
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



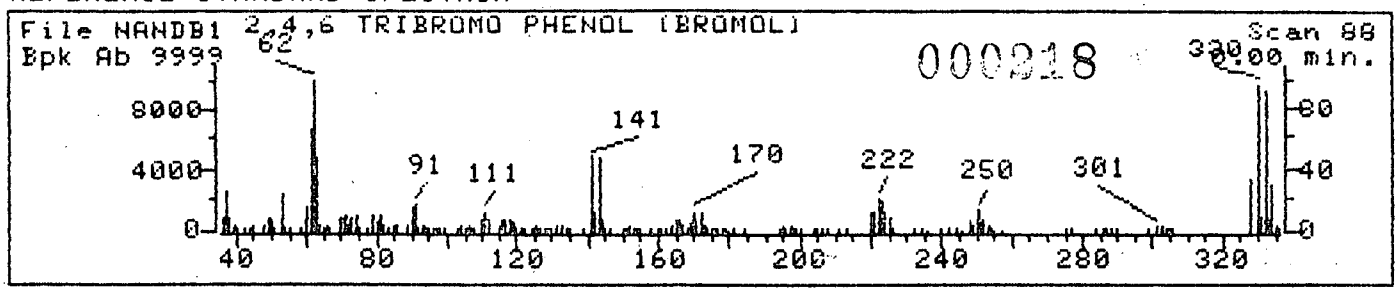
SAMPLE SPECTRUM (UNALTERED)



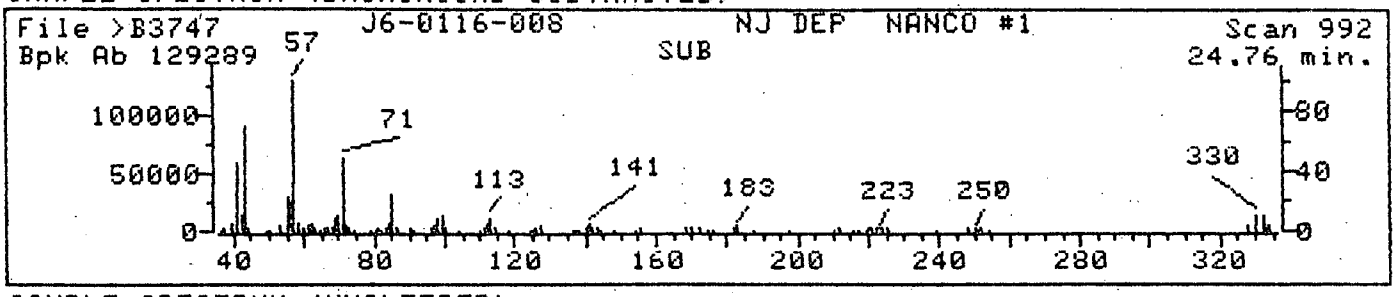
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 78
Compound Name: 2-Fluorobiphenyl (Surr)
Scan Number: 771
Retention Time: 20.25 min.
Area: 243647
Concentration: ~~2683.07 UG~~ 50
q-value: 98
86.49

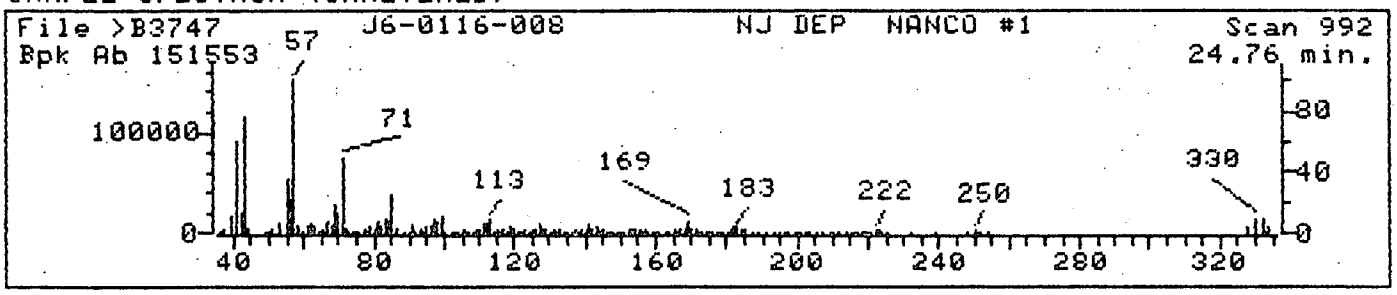
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



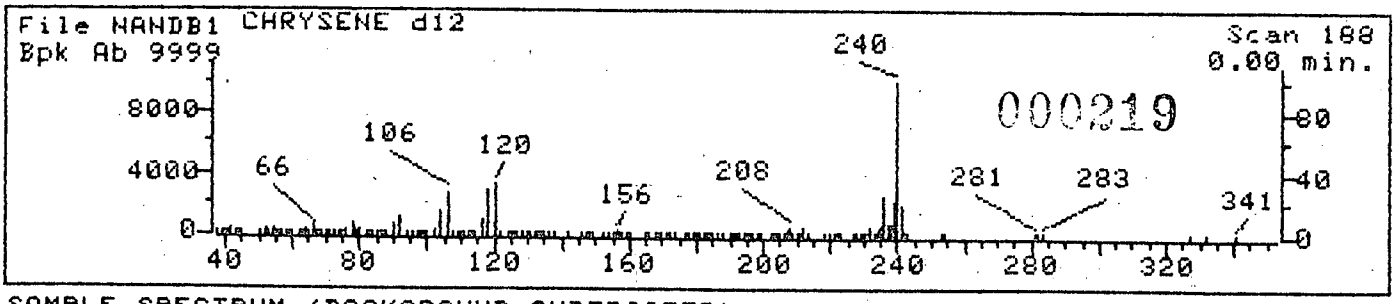
Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 79
Compound Name: 2,4,6-Tribromophenol(Surr)
Scan Number: 992
Retention Time: 24.76 min.
Area: 72780
Concentration: ~~3865.76~~ UG
q-value: 93

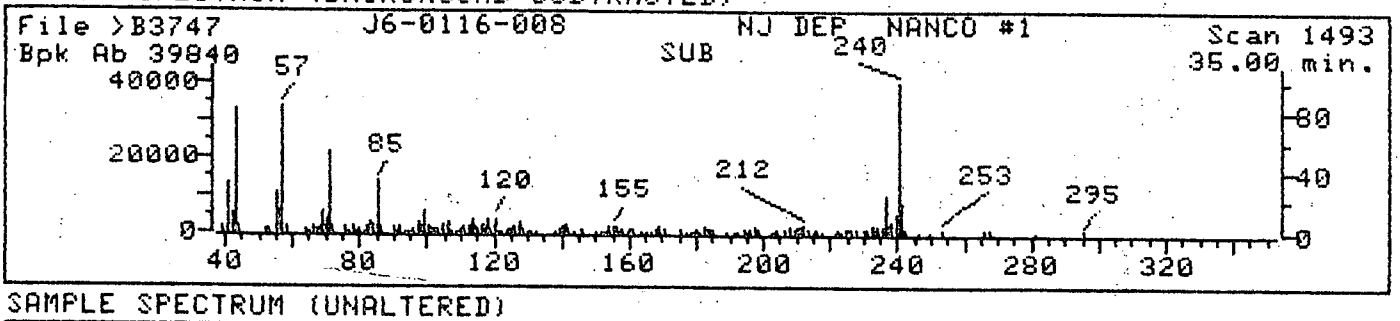
115.97

50

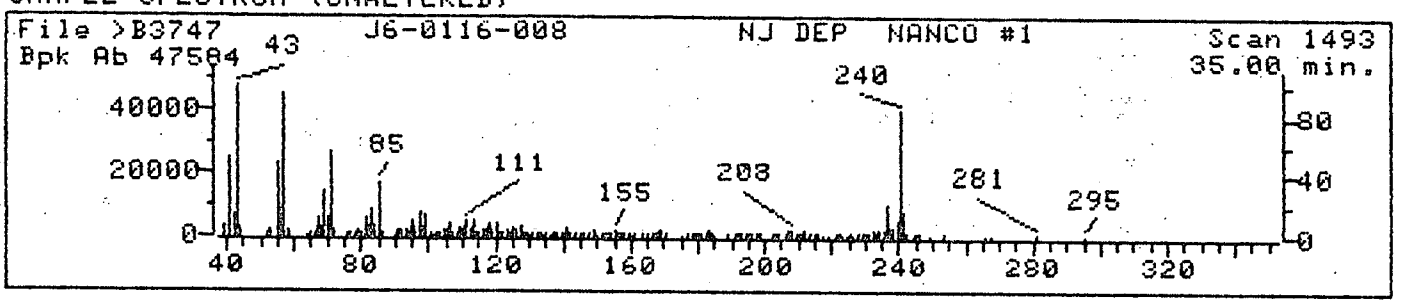
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)

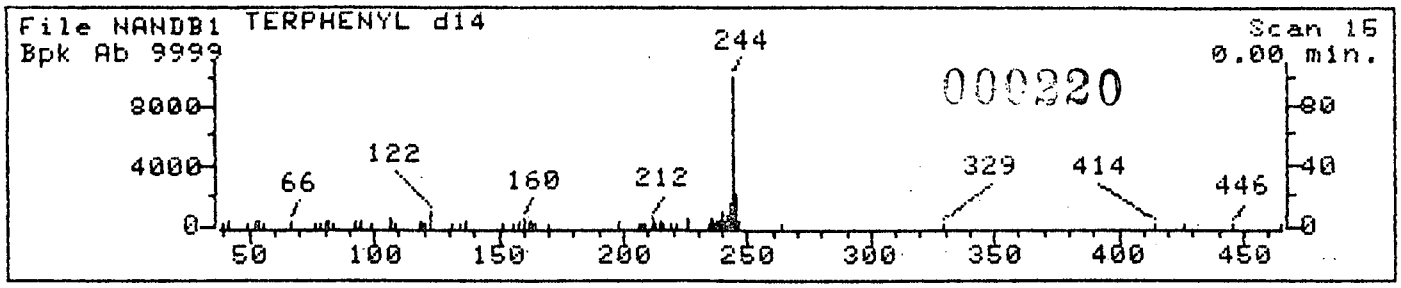


Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1
Quant Time: 861023 09:57
Injected at: 861022 18:13

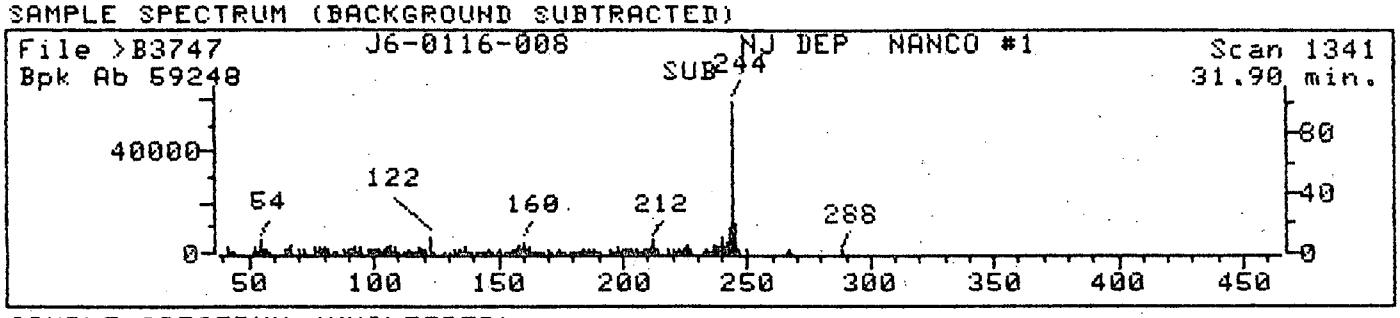
BTL# 3

Compound No: 80 (ISTD)
Compound Name: Chrysene-d12 (IS)
Scan Number: 1493
Retention Time: 35.00 min.
Area: 222019
Concentration: 40.00 UG
q-value: 100

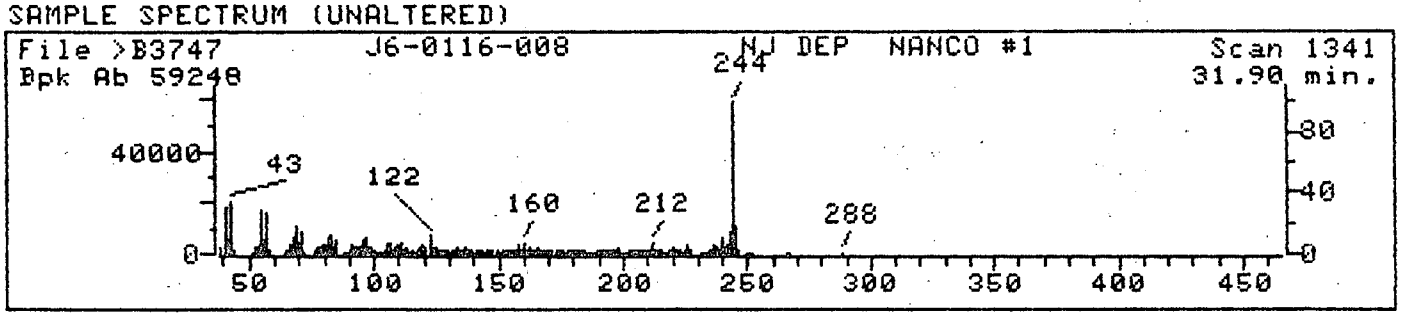
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



Data File: >B3747::D1
Name: J6-0116-008
Misc: NJ DEP NANCO #1 BTL# 3
Quant Time: 861023 09:57
Injected at: 861022 18:13

Compound No: 81
Compound Name: Terphenyl-d14 (Surr)
Scan Number: 1341
Retention Time: 31.90 min.
Area: 273494
Concentration: ~~4060.10~~ UG 50
q-value: 97
121.80

MS data file header from : >B3747

Sample: J6-0116-008 Operator: MORRIS MS 10/22/86 18:13
Misc : NJ DEP NANCO #1 BTL# 3
Sys. #: 1 MS model: 96 SW/HW rev.: IA ALS # : 0
Method file: METH01 Tuning file: MT7986 No. of extra records: 1
Source temp.: 200 Analyzer temp.: 220 Transfer line temp. : 280

Chromatographic temperatures : 30. 310. 0. 0. 0.
Chromatographic times, min. : 4.0 10.0 0.0 0.0 0.0
Chromatographic rate, deg/min: 8.0 0.0 0.0 0.0 0.0

>B3747 J6-0116-008 NJ DEP NANCO #1 000221
35.0| 500.0 TIC

Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
1	7.541	142	145	152	124044	389537	375352	4.43	.286
SR 2	9.568	241	245	252	135388	516446	497934	5.87	.380
3	11.717	347	351	354	80463	358296	334867	3.95	.256
SR 4	12.204	369	375	385	92142	599656	537687	6.34	.410
5	12.488	385	389	394	49770	241173	206295	2.43	.157
6	12.671	394	398	402	83770	314170	277478	3.27	.212
B 7	12.853	402	407	412	210523	835963	790072	9.32	.603
8	13.178	418	423	428	63479	437037	343164	4.05	.262
9	13.847	450	456	458	60089	407873	308787	3.64	.236
10	14.010	458	464	467	66935	735400	342800	4.04	.262
11	14.152	469	471	475	54863	364279	200184	2.36	.153
12	14.456	481	486	487	52619	342490	245659	2.90	.187
R 13	14.578	487	492	493	101108	820479	389602	4.59	.297
14	14.944	506	510	513	291728	1303336	1010449	11.91	.771
15	15.309	520	528	530	109936	845354	582203	6.86	.444
16	15.411	530	533	536	63442	458804	216307	2.55	.165
17	15.532	536	539	543	51034	479124	215917	2.55	.165
18	15.756	543	550	551	43458	587697	286788	3.38	.219
19	15.898	554	557	560	53045	520868	222695	2.63	.170
20	16.081	560	566	570	127140	1389670	892343	10.52	.681
21	16.304	574	577	579	92874	819598	234493	2.76	.179
22	16.426	579	583	586	85540	846880	388215	4.58	.296
IS 23	16.691	591	596	600	252252	1821743	1359240	16.03	1.037
24	16.833	600	603	607	41922	1005861	231770	2.73	.177
25	17.036	607	613	616	652813	3717377	2739150	32.30	2.090
26	17.321	620	627	629	235754	1773341	1106236	13.04	.844
27	17.565	636	639	645	95332	1321503	453767	5.35	.346
28	17.788	645	650	652	92422	1166583	490997	5.79	.375
29	18.073	659	664	667	149281	1890472	729071	8.60	.556
30	18.195	667	670	672	62287	1142071	232742	2.74	.178
31	18.297	672	675	676	82506	1175817	221881	2.62	.169
32	18.419	676	681	682	180828	2198306	722726	8.52	.552
33	18.663	691	693	698	60542	1417252	220003	2.59	.168
34	18.806	698	700	702	53802	876973	193221	2.28	.147
35	18.989	702	709	713	1001665	7081955	4972506	58.63	3.795
36	19.294	721	724	726	108178	1475156	373407	4.40	.285
37	19.416	726	730	735	130400	2556365	627930	7.40	.479
38	19.539	735	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

40	20.048	759	761	762	100930	1182125	223117	2.63	.170
41	20.129	762	765	767	176070	2358757	467839	5.52	.357
42	20.252	767	771	773	193204	3075843	571933	6.74	.436
43	20.374	773	777	779	372212	3149956	1140695	13.45	.870
44	20.435	779	780	785	83894	1792782	314839	3.71	.240
45	20.802	785	798	800	1246313	11928304	8231371	97.05	6.282
46	20.985	802	807	813	148476	4732611	1010954	11.92	.771
47	21.251	813	820	822	207650	4245386	1199117	14.14	.915
48	21.393	826	827	832	139985	2534961	325258	3.84	.248
49	21.597	832	837	842	331446	6136235	2452272	28.91	1.871
50	21.842	842	849	852	627390	7902432	2939943	34.66	2.244
51	21.964	852	855	859	150362	3744323	578045	6.82	.441
52	22.148	862	864	866	86559	1989075	192024	2.26	.147
53	22.291	866	871	872	197018	3510923	814211	9.60	.621
54	22.475	872	880	882	1311801	12069514	6626575	78.13	5.057
55	22.597	882	886	888	54323	3546743	281041	3.31	.214
56	23.026	901	907	909	135342	4566334	755150	8.90	.576
57	23.210	913	916	918	96705	3260571	477910	5.63	.365
58	23.332	918	922	925	237033	5797202	1274685	15.03	.973
59	23.577	932	934	941	201177	5237610	1001249	11.81	.764
60	24.047	944	957	958	1297145	14899218	8481152	100.00	6.472
61	24.169	958	963	966	141489	5525846	843696	9.95	.644
62	24.558	978	982	983	60083	2875294	291284	3.43	.222
63	24.762	985	992	995	687956	9412624	4293853	50.63	3.277
64	24.885	995	998	1003	256721	5875533	1819526	21.45	1.389
65	25.069	1003	1007	1009	139260	3619518	613231	7.23	.468
66	25.273	1015	1017	1021	63291	3631611	274414	3.24	.209
67	25.518	1021	1029	1030	1454515	12203994	7167990	84.52	5.470
68	25.600	1030	1033	1036	1075522	7410366	4020726	47.41	3.068
69	25.804	1040	1043	1046	96589	3832955	424202	5.00	.324
70	26.111	1053	1058	1061	220440	5709120	1306571	15.41	.997
71	26.213	1061	1063	1066	134957	3529807	576002	6.79	.440
72	26.377	1069	1071	1075	146406	4141233	402563	4.75	.307
73	26.888	1089	1096	1098	1029439	11152826	5881394	69.35	4.488
74	27.031	1098	1103	1106	729291	7463722	2891976	34.10	2.207
75	27.358	1116	1119	1121	68071	3111135	324012	3.82	.247
76	27.440	1121	1123	1131	163616	6340705	851249	10.04	.650
77	27.665	1131	1134	1135	84531	2487884	316128	3.73	.241
78	27.706	1135	1136	1140	109504	3210007	516930	6.10	.394
79	27.828	1140	1142	1144	134185	2484841	355994	4.20	.272
80	28.217	1150	1161	1164	998617	12652736	5186672	61.16	3.958
81	28.380	1164	1169	1171	74769	4176433	443152	5.23	.338
82	28.707	1182	1185	1187	87158	3022929	369699	4.36	.282
83	29.096	1202	1204	1208	58514	3271193	214258	2.53	.164
84	29.464	1216	1222	1225	906096	8201532	3907901	46.08	2.982
85	29.934	1241	1245	1253	126383	6080174	985335	11.62	.752
86	30.220	1253	1259	1261	110358	4066349	669843	7.90	.511
87	30.343	1262	1265	1266	62037	2199563	221046	2.61	.169
88	30.670	1275	1281	1283	674647	5884564	2611468	30.79	1.993
89	31.120	1296	1303	1308	108247	5441137	1025952	12.10	.783
90	31.610	1325	1327	1332	78462	2796582	324918	3.83	.248
91	31.815	1332	1337	1339	519045	4568388	2094153	24.69	1.598
92	31.897	1339	1341	1345	179074	2735952	547166	6.45	.418
93	32.224	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]

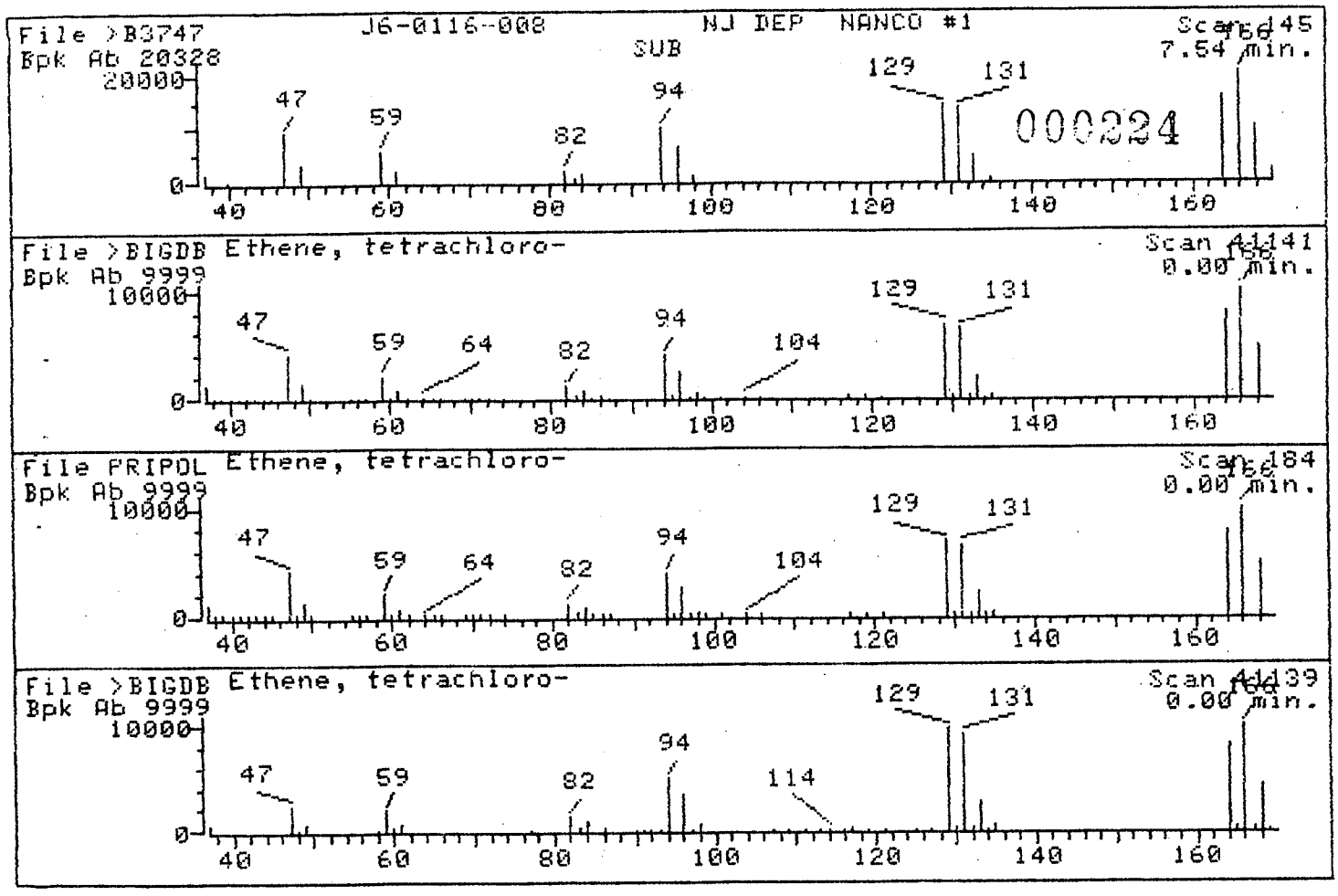
000222

95	33.307	1407	1410	1419	55945	3591732	392951	4.63	.300
96	33.981	1436	1443	1446	229773	3467053	844956	9.96	.645
S 97	35.001	1488	1493	1502	320206	4907656	1624070	19.15	1.239
98 H	35.572	1513	1521	1526	306769	4668889	1392854	16.42	1.063
99	36.001	1537	1542	1550	218468	4108703	983517	11.60	.751
100	36.327	1555	1558	1563	37368	2275752	266742	3.15	.204
101	36.552	1565	1569	1576	66218	3310621	536523	6.33	.409
102	36.960	1585	1589	1594	158238	2825667	630123	7.43	.481
103 H	37.368	1605	1609	1614	185357	3074163	723954	8.54	.552
104	37.878	1631	1634	1638	129577	2411743	447537	5.28	.342
105	38.449	1658	1662	1665	63990	2387651	328305	3.87	.251
106	38.775	1674	1678	1682	145941	3071546	545444	6.43	.416
107	39.163	1690	1697	1708	266588	7452185	1853012	21.85	1.414
108	39.429	1708	1710	1718	58867	3192638	480514	5.67	.367
109	39.673	1719	1722	1731	136057	3539395	652580	7.69	.498
110	39.979	1735	1737	1745	36630	2370754	219507	2.59	.168
111	40.244	1747	1750	1757	36596	2243388	240896	2.84	.184
112	40.672	1767	1771	1776	82881	1915991	365852	4.31	.279
113	41.120	1789	1793	1800	82905	2097767	422868	4.99	.323
114	41.792	1822	1826	1830	43525	1265706	215025	2.54	.164

Sum of corrected areas: 131039200.

000223

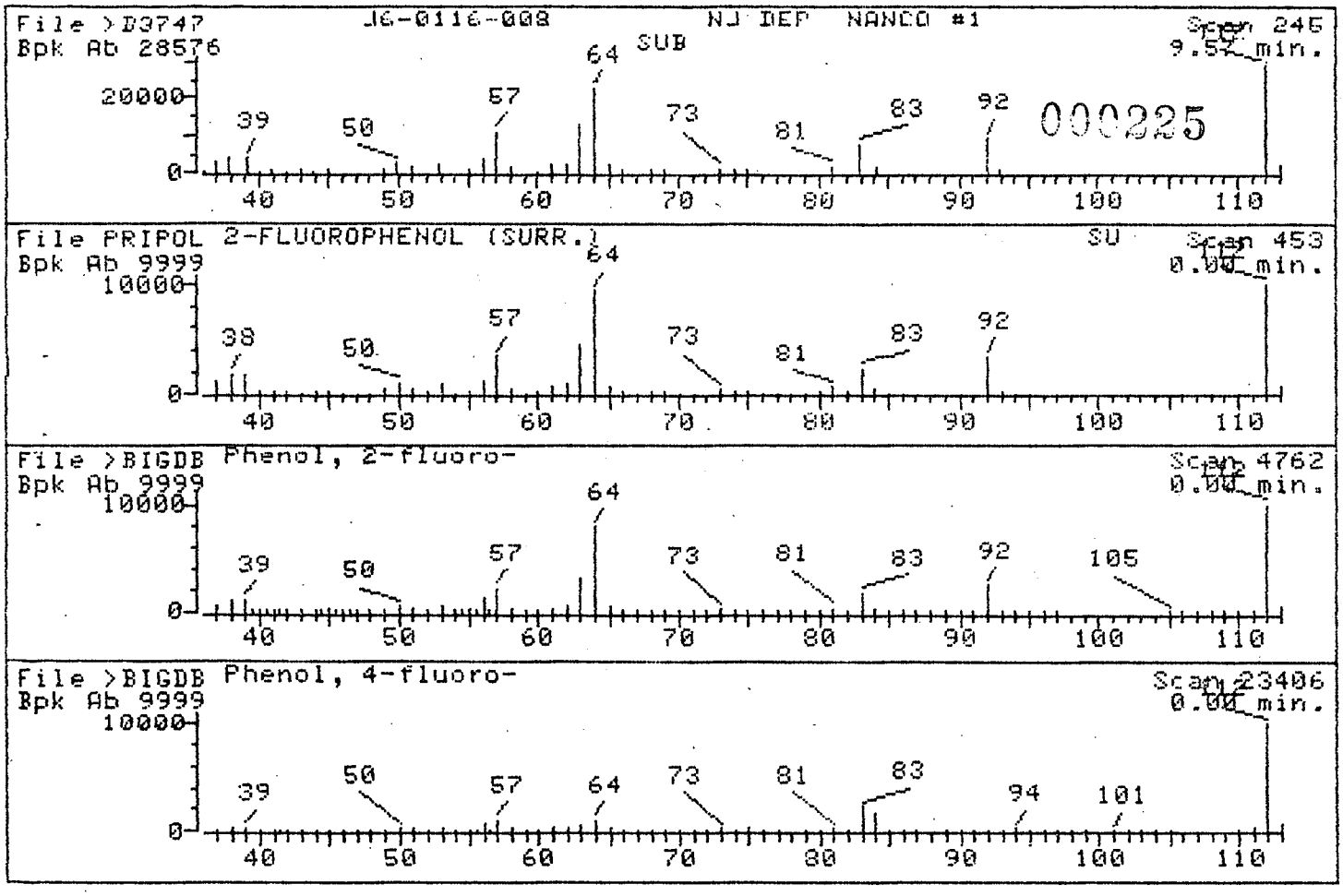
Use PK #7 (DSTD) for all TICS Calculations



1. Ethene, tetrachloro- 164 C2Cl4
2. Ethene, tetrachloro- 164 C2Cl4
3. Ethene, tetrachloro- 164 C2Cl4
4. Ethene, tetrachloro- 164 C2Cl4
5. Ethene, tetrachloro- 164 C2Cl4

Sample file: >B3747 Spectrum #: 145
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	95*	127184	41141	"BIGDB	115	28	2	0	97	0	72	93
2.	95*	184	283	PRIPOL	115	28	2	0	97	0	72	93
3.	83*	127184	41139	"BIGDB	82	49	1	0	68	12	51	78
4.	83*	182	281	PRIPOL	82	49	1	0	68	12	51	78
5.	74*	181	280	PRIPOL	67	55	2	0	96	14	39	46

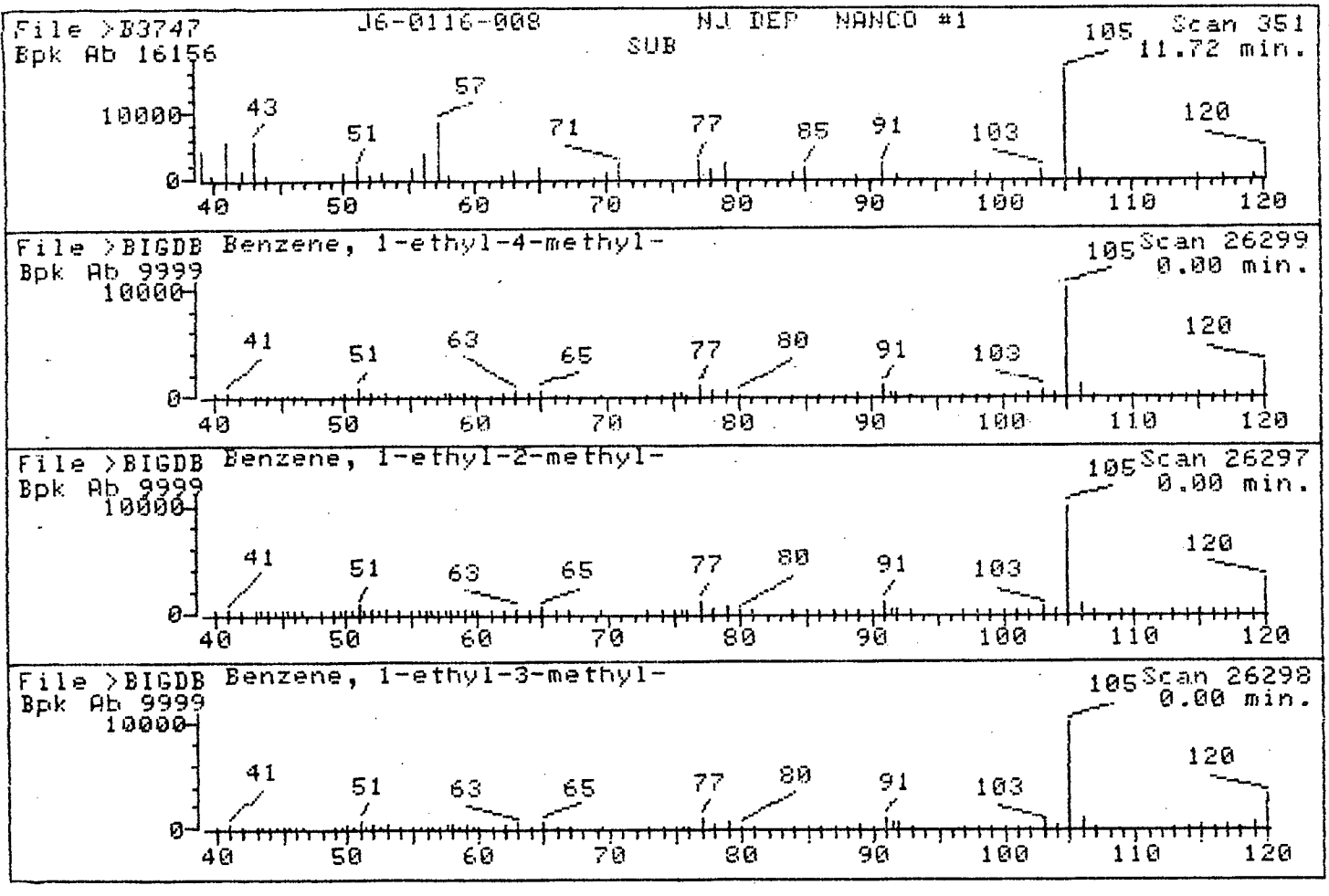


1. 2-FLUOROPHENOL (SURR.) SU 112 C6.H5FO
   RROGATE COMPOUND BNA
   SURROGATE
2. Phenol, 2-fluoro- 112 C6H5FO
3. Phenol, 4-fluoro- 112 C6H5FO
4. Phenol, 3-fluoro- 112 C6H5FO
5. 1H-Tetrazaborole, 4,5-dihydro-1,4,5-trimethyl- 112 C3H9BN4

16

Sample file: >B3747 Spectrum #: 245
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	99*	453	57	PRIPOL	114	2	0	0	77	0	72	99
2.	97*	367124	4762	"BIGDB	95	14	0	0	98	1	72	97
3.	25*	371415	23406	"BIGDB	32	58	2	0	100	50	7	16
4.	25*	372203	23405	"BIGDB	34	66	2	0	74	46	7	14
5.	15*	20546183	23379	"BIGDB	26	71	3	0	100	60	3	13

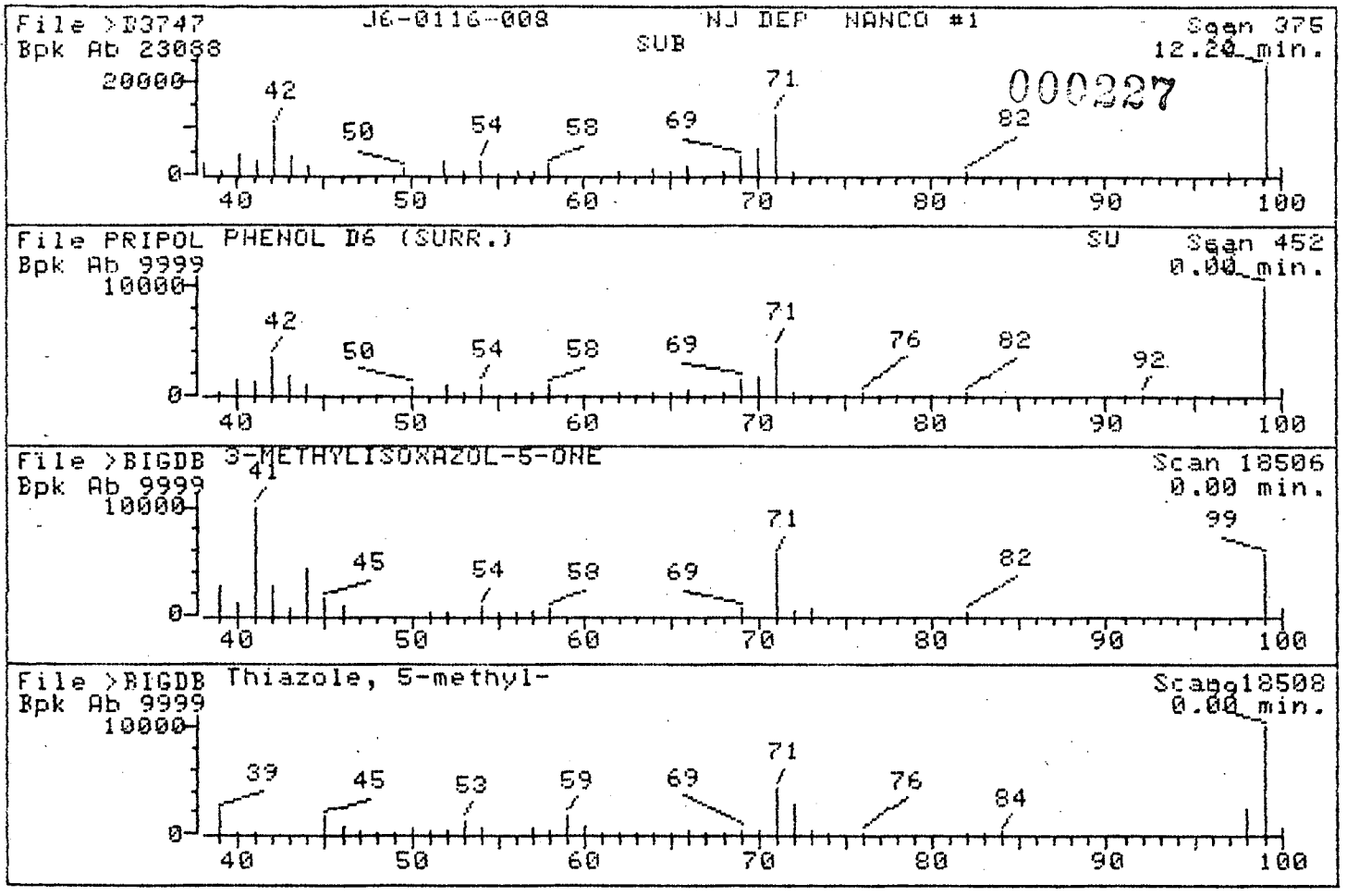


000226

1.	Benzene, 1-ethyl-4-methyl-	120	C9H12
2.	Benzene, 1-ethyl-2-methyl-	120	C9H12
3.	Benzene, 1-ethyl-3-methyl-	120	C9H12
4.	Benzene, (1-methylethyl)-	120	C9H12
5.	Benzene, (1-methylethyl)-	120	C9H12

Sample file: >B3747 Spectrum #: 351
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	64*	622968	26299	"BIGDB	58	27	2	0	88	24	28	44
2.	59*	611143	26297	"BIGDB	52	33	2	0	85	24	27	35
3.	59*	620144	26298	"BIGDB	49	38	2	0	80	24	27	30
4.	58*	98828	26592	"BIGDB	55	38	2	0	75	30	24	38
5.	53*	98828	26293	"BIGDB	51	36	2	0	88	30	24	33

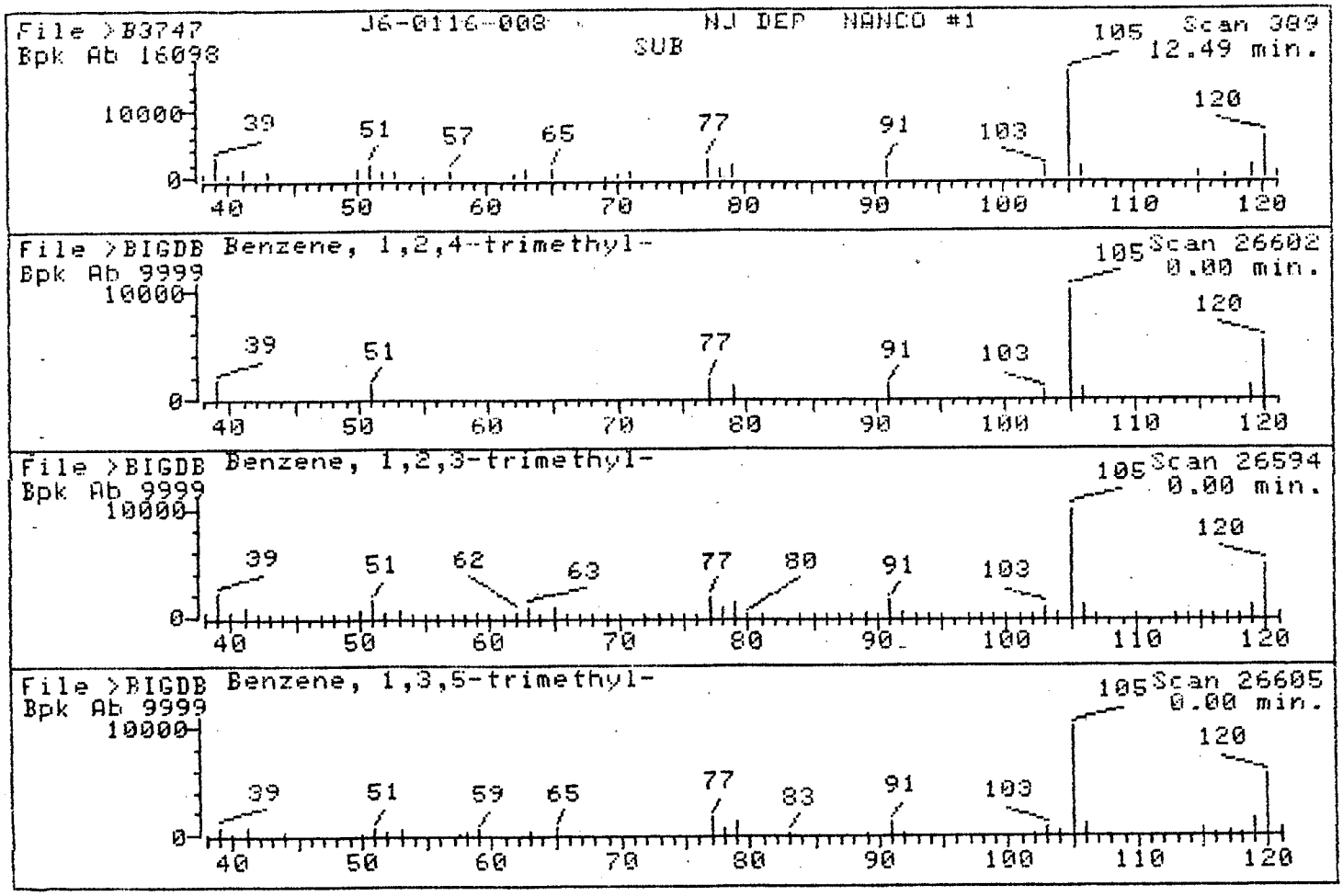


16

1.	PHENOL D6 (SURR.) RROGATE COMPOUND ~~SURROGATE~~	SU BNA	100 C6.D6.0
2.	3-METHYLISOXAZOL-5-ONE		99 C4H5NO2
3.	Thiazole, 5-methyl-		99 C4H5NS
4.	3,4-DIAMINO-1,2,4-TRIAZOLE		99 C2H5N5
5.	2,5-Pyrrolidinedione		99 C4H5NO2

Sample file: >B3747 Spectrum #: 375
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	83	452	159	PRIPOL	77	17	2	0	100	0	57	28
2.	25*	1517960	18506	"BIGDB	27	70	3	0	102	46	7	13
3.	24*	3581893	18508	"BIGDB	23	87	3	0	100	44	8	12
4.	20*	0	18500	"BIGDB	22	35	3	0	100	55	5	12
5.	20*	123568	18505	"BIGDB	27	56	2	0	100	55	5	14

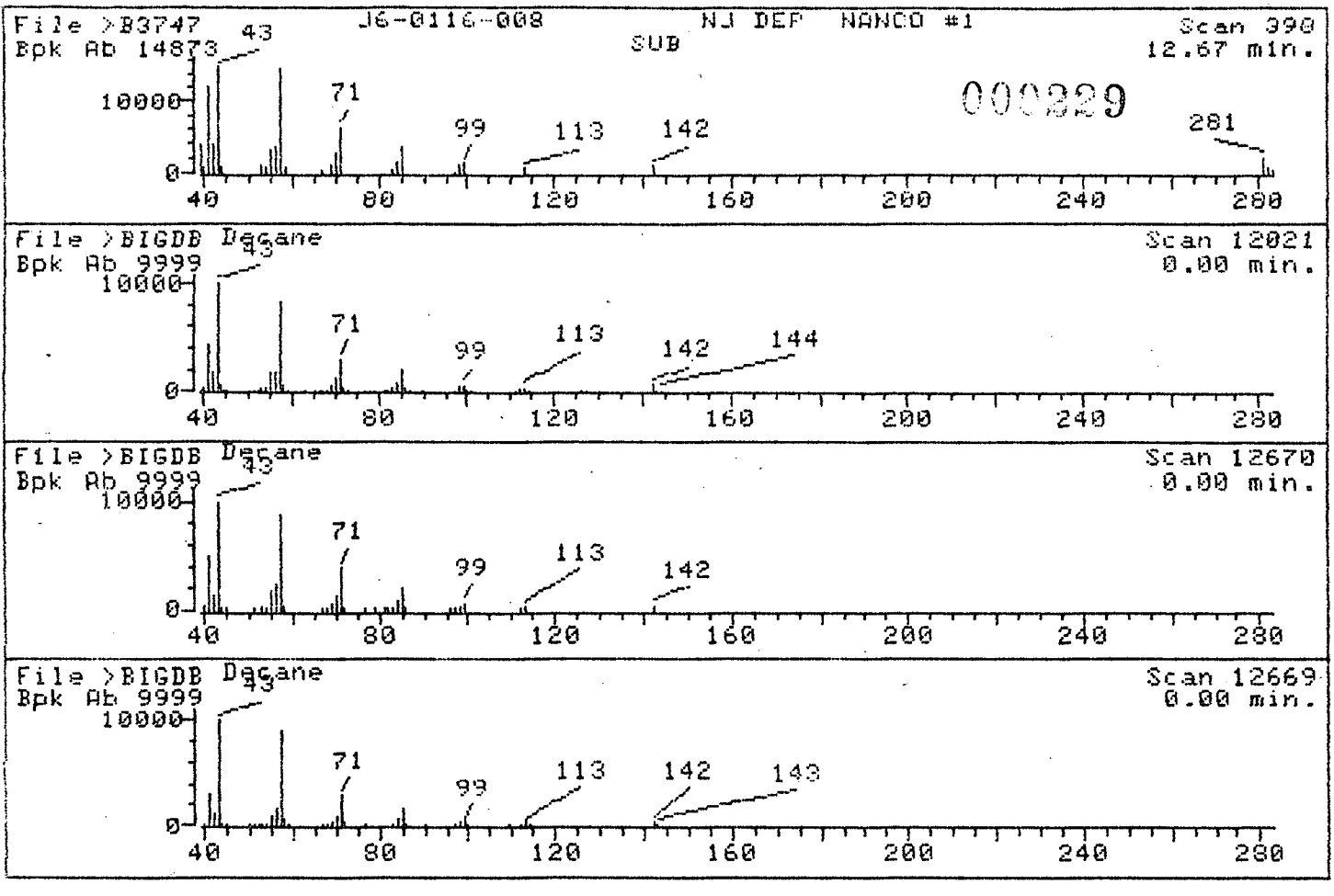


000228

1. Benzene, 1,2,4-trimethyl- 120 C9H12
2. Benzene, 1,2,3-trimethyl- 120 C9H12
3. Benzene, 1,3,5-trimethyl- 120 C9H12
4. Benzene, 1,2,4-trimethyl- 120 C9H12
5. Benzene, 1,2,3-trimethyl- 120 C9H12

Sample file: >B3747 Spectrum #: 389
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

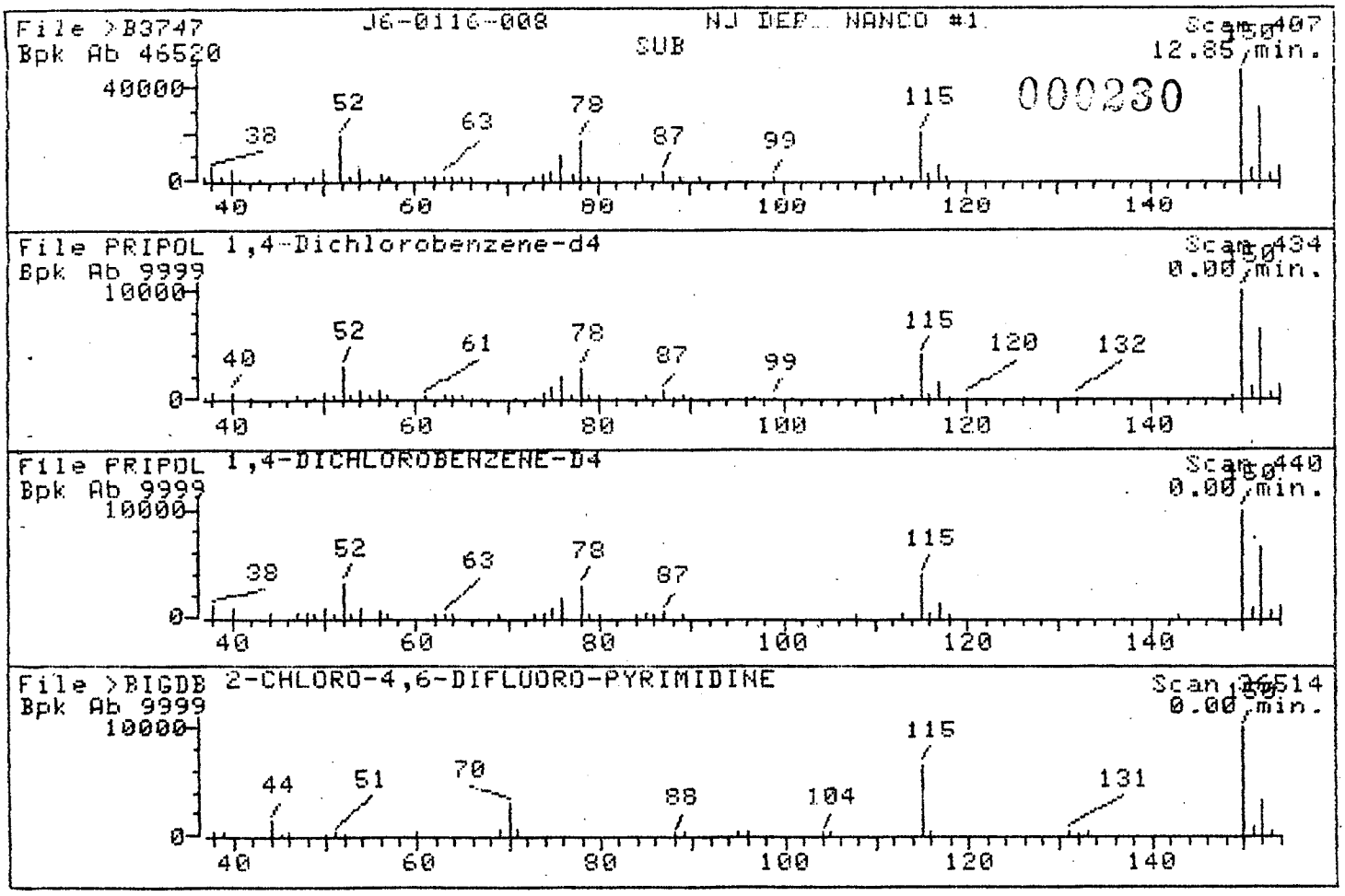
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	96*	95636	26602	"BIGDB	64	5	0	0	72	3	72	96
2.	88*	526738	26594	"BIGDB	74	26	2	0	79	0	65	56
3.	81*	108678	26605	"BIGDB	66	29	2	0	69	6	53	49
4.	81*	95636	26599	"BIGDB	62	30	2	0	76	6	53	49
5.	81*	526738	26294	"BIGDB	62	30	2	0	70	6	53	49



1. Decane	142	C10H22
2. Decane	142	C10H22
3. Decane	142	C10H22
4. Decane	142	C10H22
5. Dodecane	170	C12H26

Sample file: >B3747 Spectrum #: 398
Search speed: 1 Tilting option: N No. of ion ranges searched: 46

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	84*	124185	12021	"BIGDB	79	18	2	0	100	6	55	67
2.	76*	124185	12670	"BIGDB	75	24	2	0	96	11	40	57
3.	74*	124185	12669	"BIGDB	60	33	2	0	109	11	39	44
4.	67	124185	12668	"BIGDB	67	33	2	0	100	11	34	23
5.	67	112403	12727	"BIGDB	60	37	2	0	88	13	34	21



J 16

1. 1,4-Dichlorobenzene-d4 150 C6.D4.CL4

2. 1,4-DICHLOROBENZENE-D4 150 C6.D4.CL4

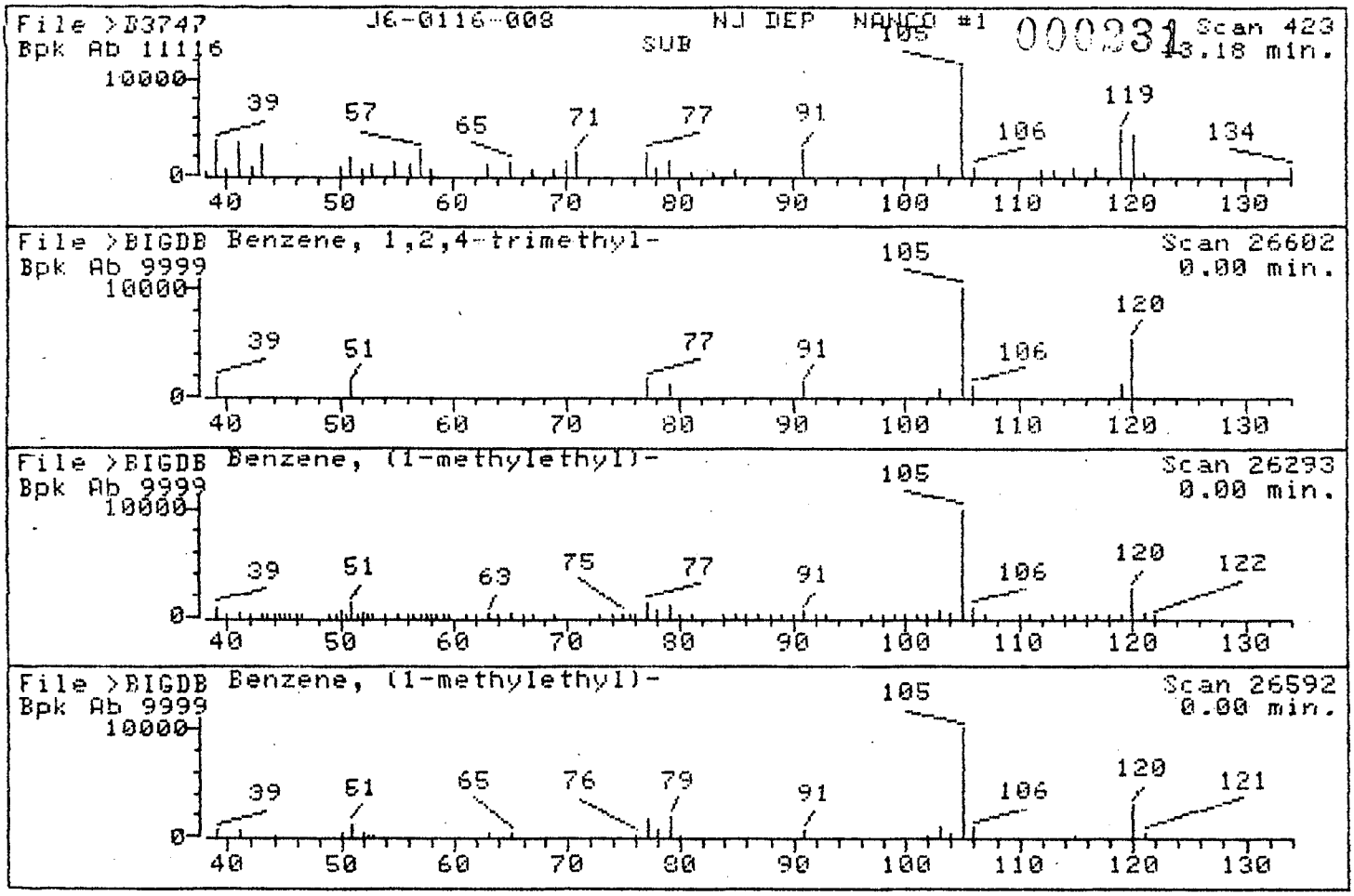
BNA

INTERNAL STD.

*3. 2-CHLORO-4,6-DIFLUORO-PYRIMIDINE 150 C4HC1F2N2

Sample file: >B3747 Spectrum #: 407
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

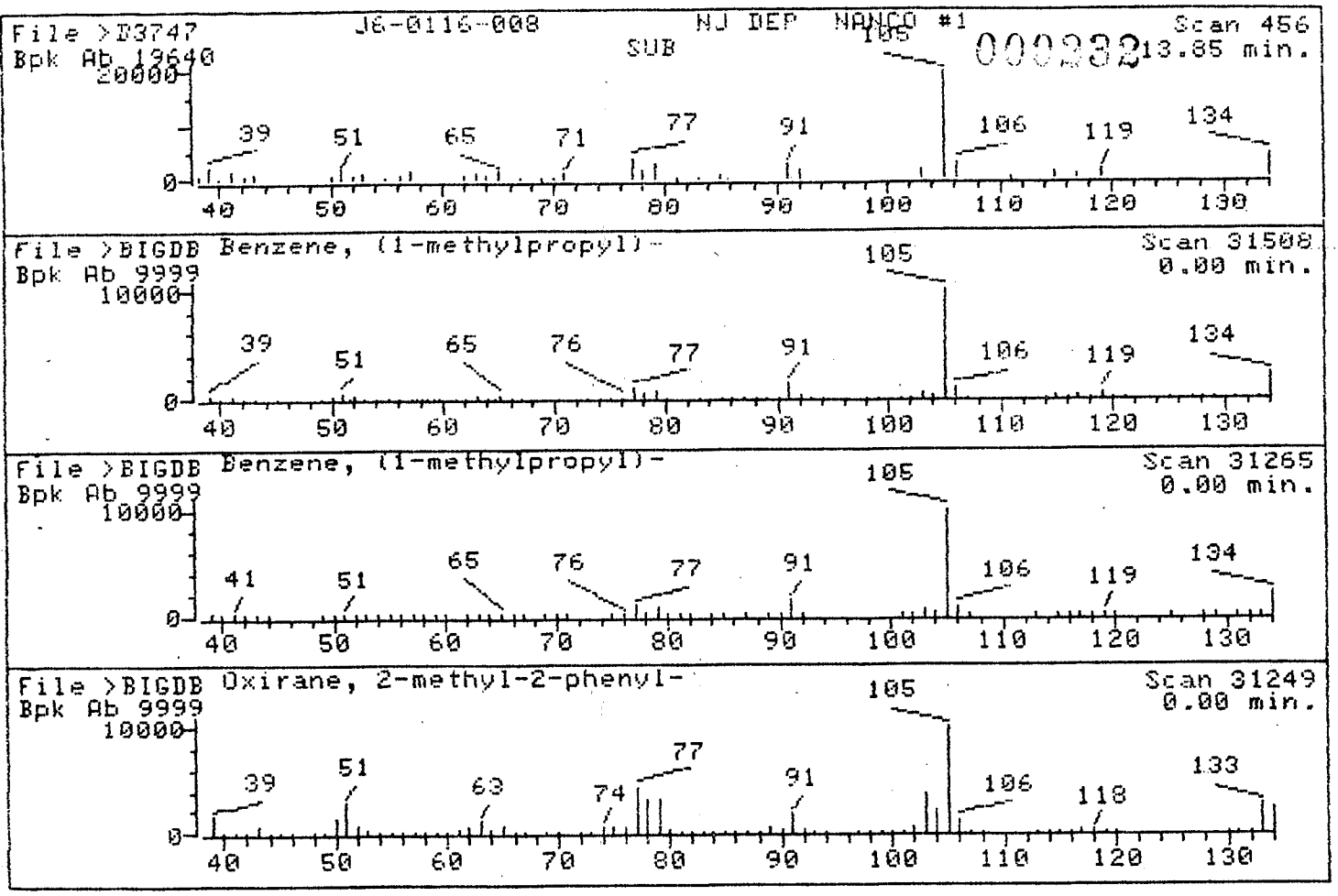
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	87*	434	256	PRIPOL	83	24	1	0	81	12	55	80
2.	81*	440	257	PRIPOL	71	39	1	0	79	16	45	71
3.	25*	38953309	36514	"BIGDB	28	67	3	0	66	45	8	13



1. Benzene, 1,2,4-trimethyl- 120 C9H12
2. Benzene, (1-methylethyl)- 120 C9H12
3. Benzene, (1-methylethyl)- 120 C9H12
4. Benzene, 1,2,3-trimethyl- 120 C9H12
5. Benzene, 1-ethyl-2-methyl- 120 C9H12

Sample file: >B3747 Spectrum #: 423
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

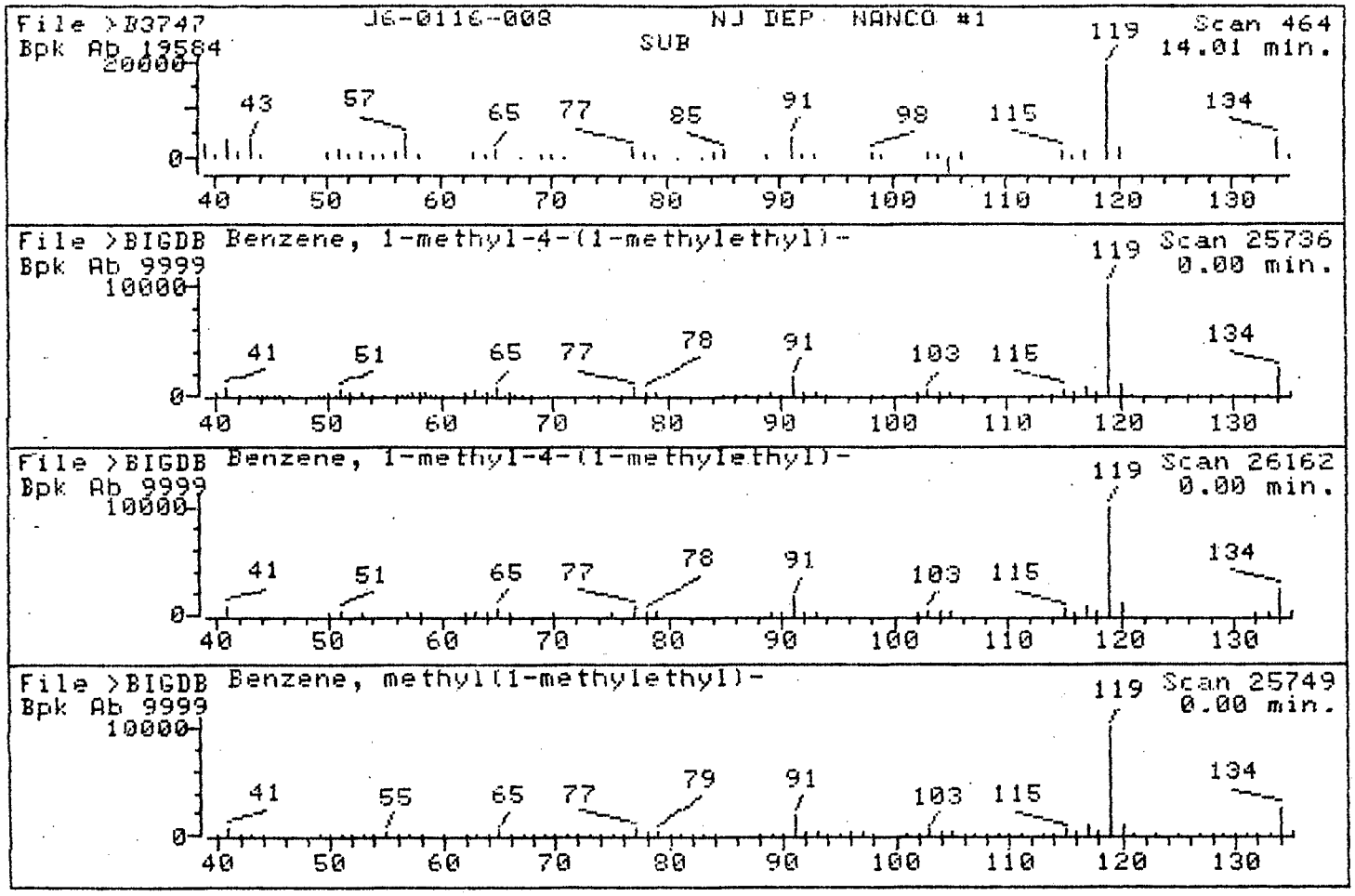
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	41*	95636	26602	"BIGDB	34	35	0	0	70	42	14	33
2.	32*	98828	26293	"BIGDB	44	43	2	0	100	42	12	23
3.	31*	98828	26592	"BIGDB	46	47	3	0	100	38	10	17
4.	30*	526738	26594	"BIGDB	42	58	2	0	78	39	10	16
5.	29*	611143	26297	"BIGDB	30	55	2	0	100	40	10	15



1. Benzene, (1-methylpropyl)- 134 C10H14
2. Benzene, (1-methylpropyl)- 134 C10H14
3. Oxirane, 2-methyl-2-phenyl- 134 C9H10O
4. Benzene, (1-methylpropyl)- 134 C10H14
5. Benzene, 1-methyl-3-propyl- 134 C10H14

Sample file: >B3747 Spectrum #: 456
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	79*	135988	31508	"BIGDB	54	31	2	0	100	8	48	39
2.	76*	135988	31265	"BIGDB	48	35	2	0	97	10	45	28
3.	70*	2085883	31249	"BIGDB	22	92	3	0	100	8	42	12
4.	67*	135988	31509	"BIGDB	47	39	2	0	100	11	34	27
5.	63*	1074437	31269	"BIGDB	49	38	2	0	92	16	30	30

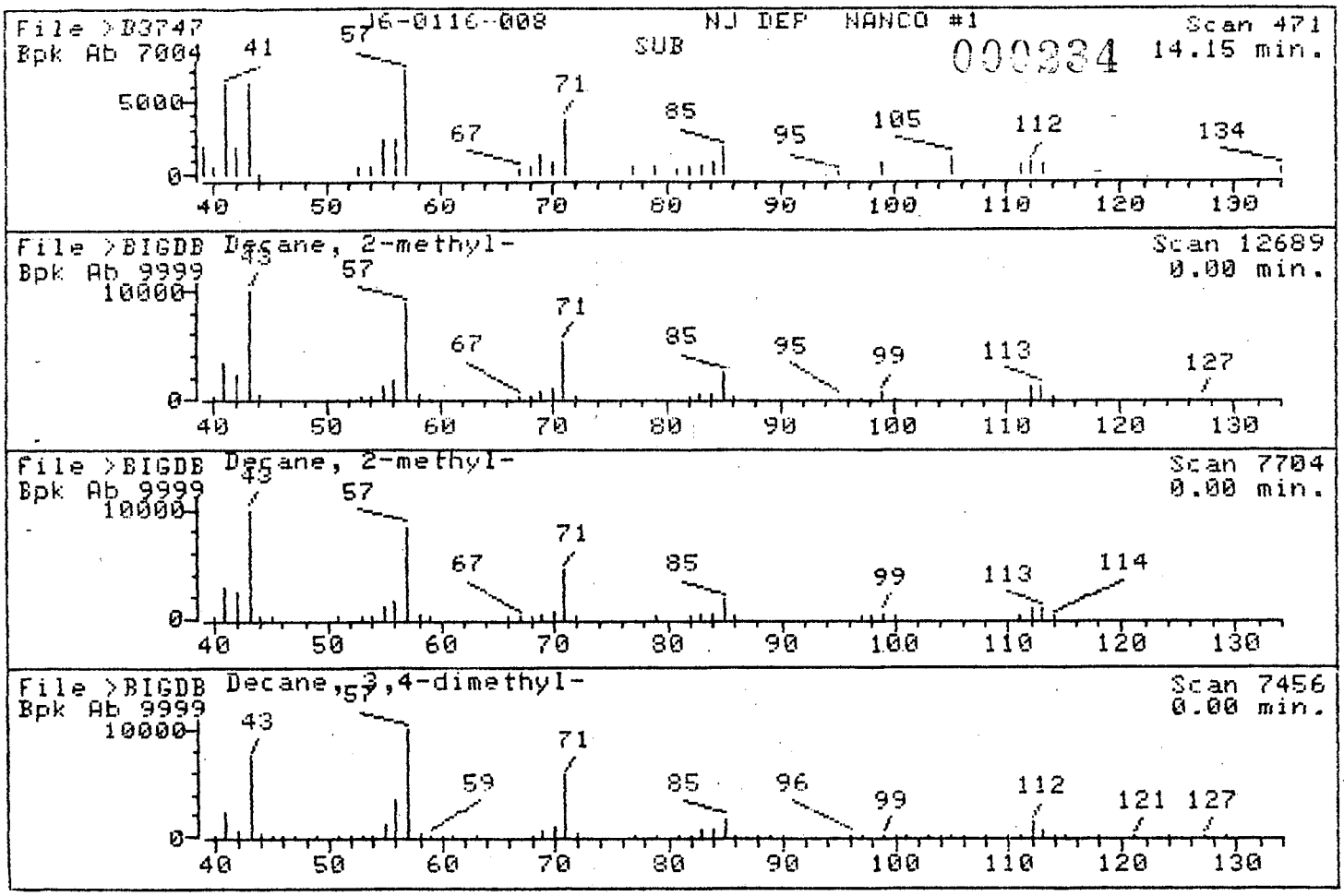


000233

1. Benzene, 1-methyl-4-(1-methylethyl)- 134 C10H14
2. Benzene, 1-methyl-4-(1-methylethyl)- 134 C10H14
3. Benzene, methyl(1-methylethyl)- 134 C10H14
4. Benzene, 1-methyl-3-(1-methylethyl)- 134 C10H14
5. Benzene, 1-methyl-4-(1-methylethyl)- 134 C10H14

Sample file: >B3747 Spectrum #: 464
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

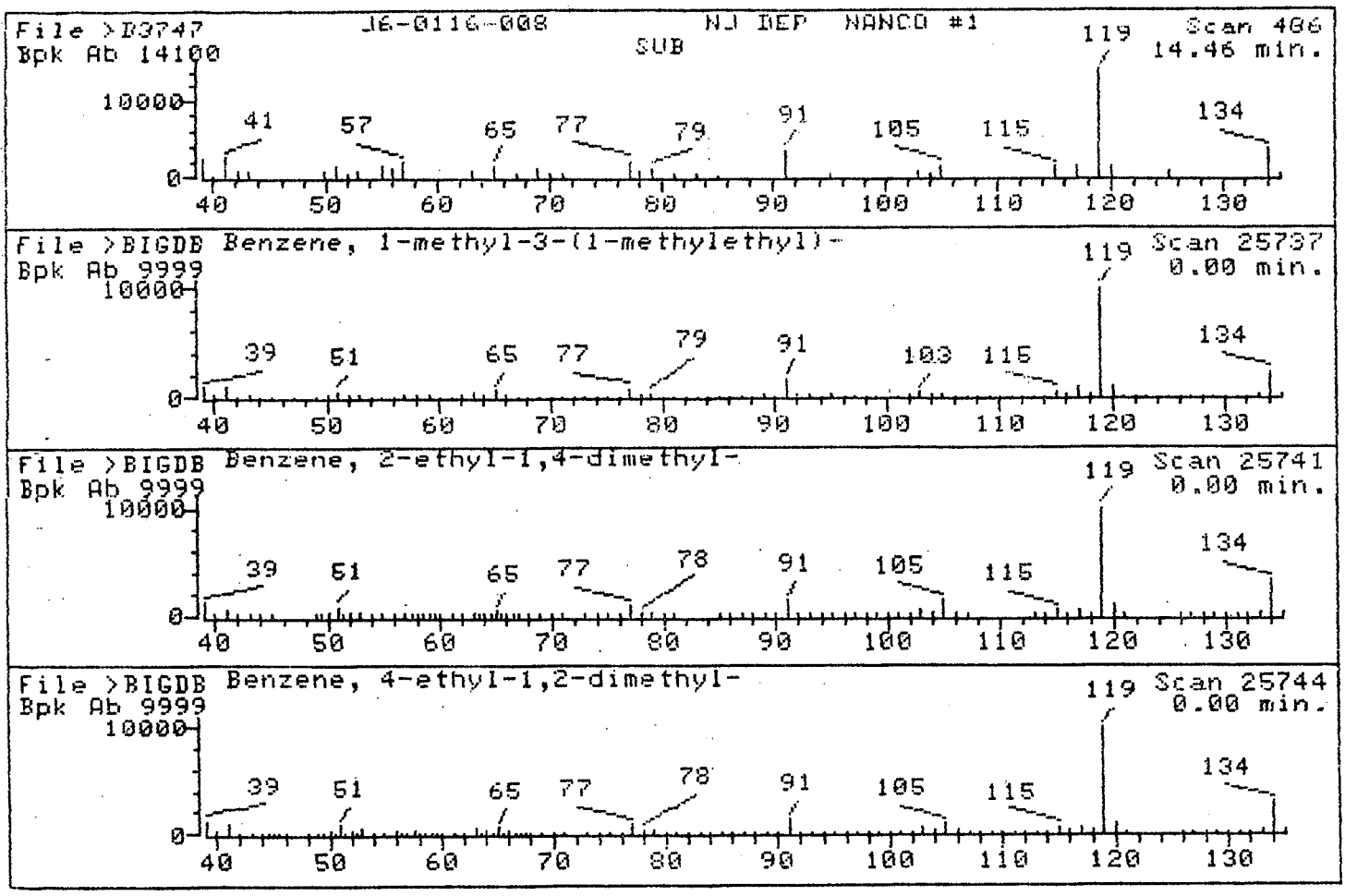
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	86*	99876	25736	"BIGDB	78	11	2	0	92	10	59	72
2.	84*	99876	26162	"BIGDB	73	16	2	0	87	10	55	66
3.	84*	25155151	25749	"BIGDB	73	17	2	0	86	10	55	66
4.	84*	535773	25737	"BIGDB	68	21	2	0	95	10	55	60
5.	83*	99876	26159	"BIGDB	63	27	2	0	91	10	54	50



1.	Decane, 2-methyl-	156 C11H24
2.	Decane, 2-methyl-	156 C11H24
3.	Decane, 3,4-dimethyl-	170 C12H26
4.	Nonane, 3-methyl-	142 C10H22
5.	1-Pentene, 2,4,4-trimethyl-	112 C8H16

Sample file: >B3747 Spectrum #: 471
Search speed: 1 Tilting option: N No. of ion ranges searched: 47

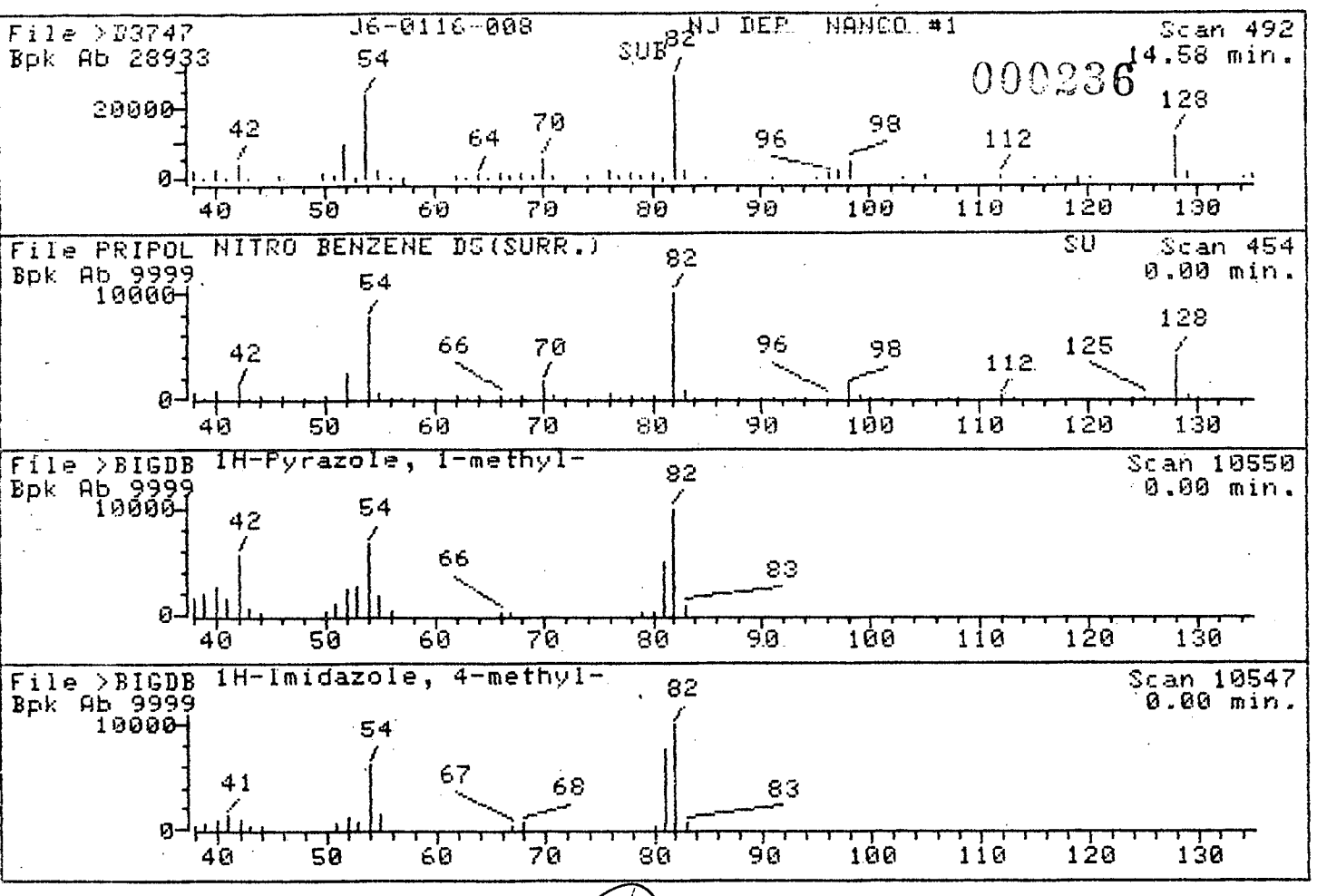
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	60	6975980	12689	"BIGDB	54	49	2	0	84	12	30	12
2.	52	6975980	7704	"BIGDB	46	48	2	0	87	16	20	12
3.	46	17312457	7456	"BIGDB	54	40	2	0	83	21	17	17
4.	42	5911046	7679	"BIGDB	40	46	2	0	100	24	17	13
5.	25*	107391	23449	"BIGDB	24	61	3	0	100	50	7	12



1.	Benzene, 1-methyl-3-(1-methylethyl)-	134	C10H14
2.	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14
3.	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14
4.	Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14
5.	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14

Sample file: >B3747 Spectrum #: 486
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	81*	535773	25737	"BIGDB	59	30	2	0	100	10	53	45
2.	81*	1758889	25741	"BIGDB	59	35	2	0	76	9	53	43
3.	81*	934805	25744	"BIGDB	57	36	2	0	87	6	53	41
4.	79*	874419	25740	"BIGDB	51	38	2	0	87	9	48	33
5.	79*	2870044	25742	"BIGDB	50	38	2	0	86	9	48	31



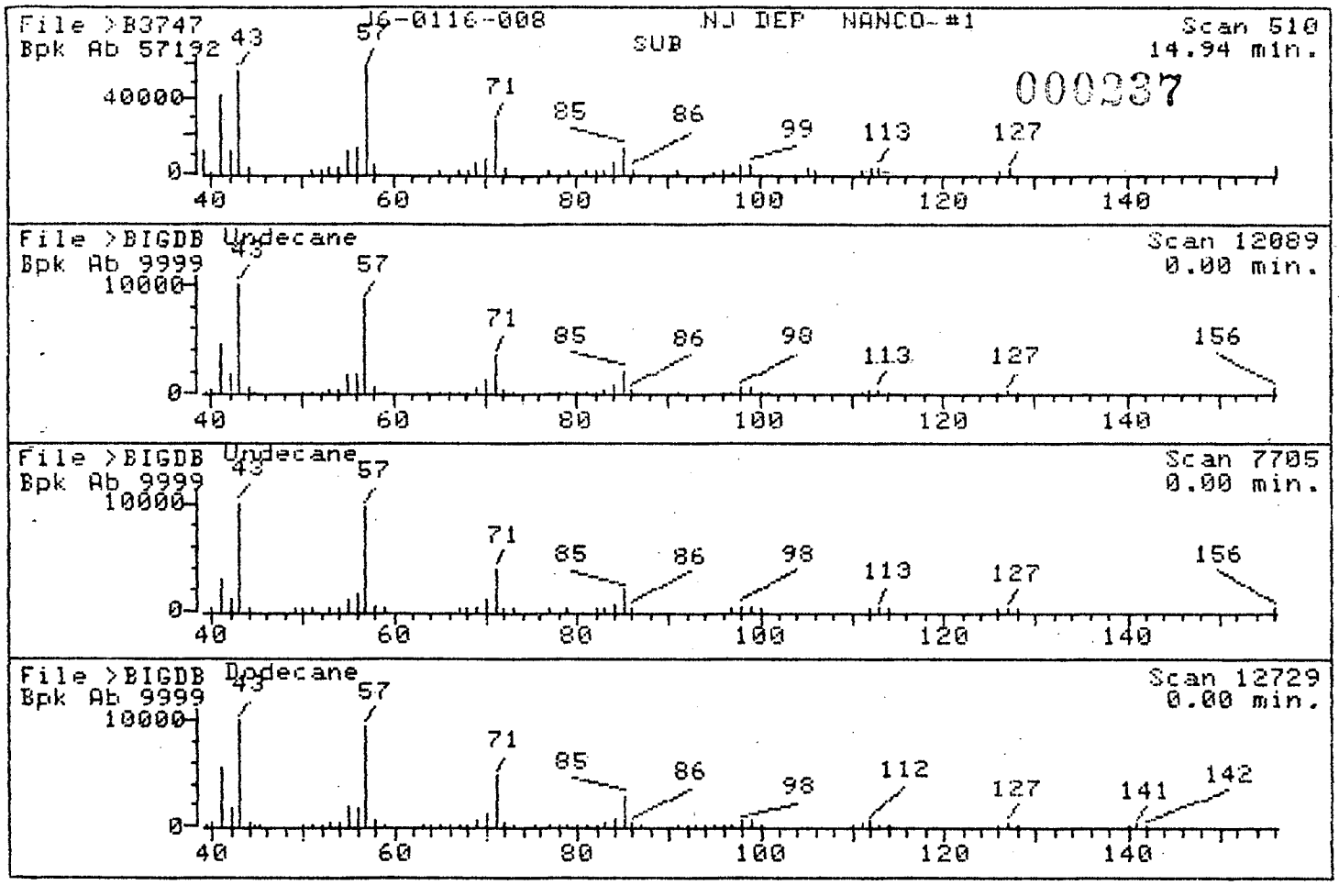
56

15 R

1. NITRO BENZENE D5(SURR.) — SU 128
   RROGATE COMPOUND — BNA
   SURROGATE
2. 1H-Pyrazole, 1-methyl- — 82 C4H6N2
3. 1H-Imidazole, 4-methyl- — 82 C4H6N2
4. 1H-Imidazole, 4-methyl- — 82 C4H6N2
5. 1H-Pyrazole, 3-methyl- — 82 C4H6N2

Sample file: >B3747 Spectrum #: 492
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

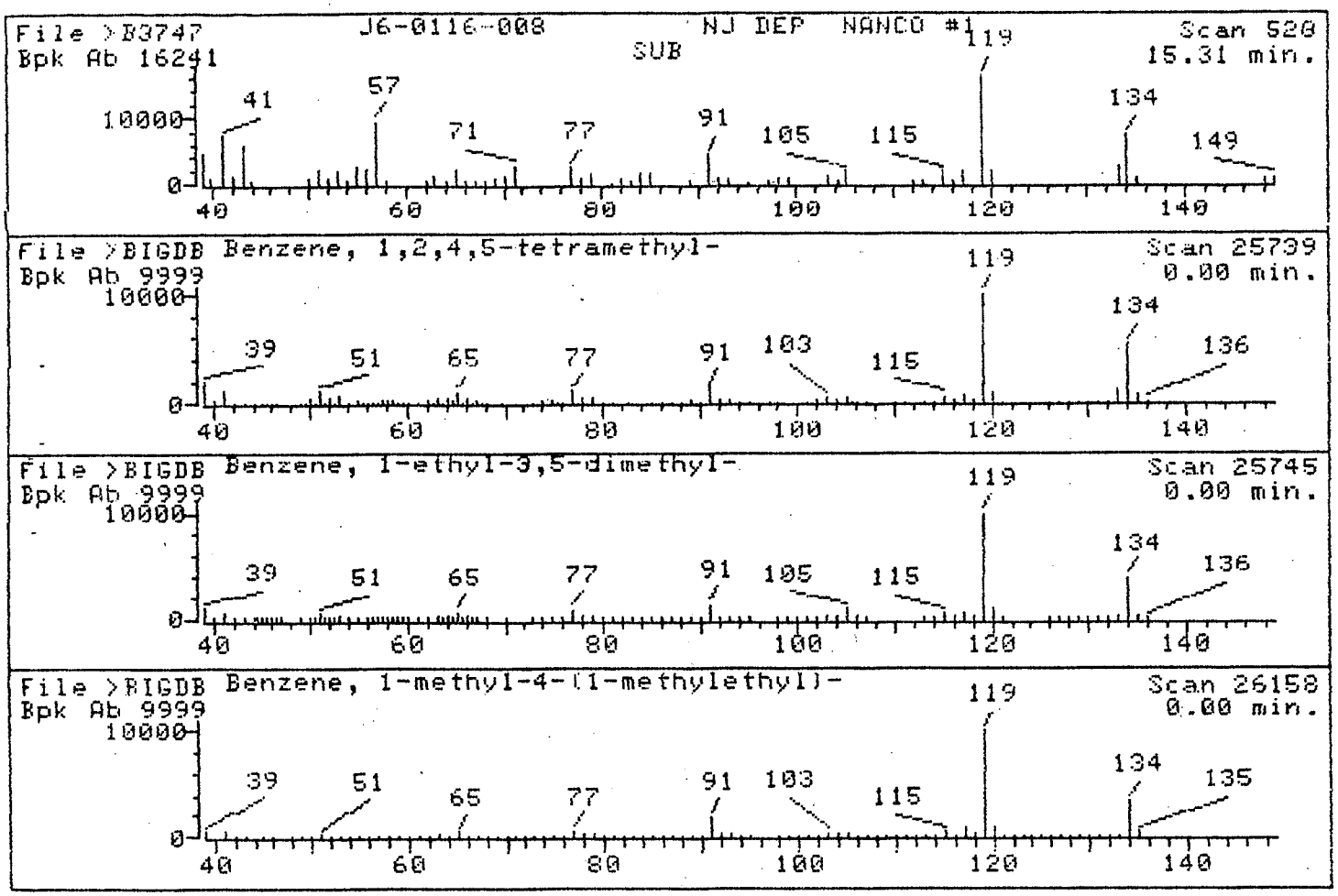
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	97*	454	15	PRIPOL	103	0	0	0	99	1	72	97
2.	36*	930369	10550	"BIGDB	26	95	3	0	100	30	14	13
3.	30*	822366	10547	"BIGDB	26	65	3	0	100	33	12	13
4.	30*	822366	10681	"BIGDB	28	68	3	0	100	33	12	13
5.	15*	1453583	10683	"BIGDB	24	66	3	0	100	57	3	12



1. Undecane	156	C11H24
2. Undecane	156	C11H24
3. Dodecane	170	C12H26
4. Tridecane	184	C13H28
5. Decane, 2-methyl-	156	C11H24

Sample file: >B3747 Spectrum #: 510
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	95*	1120214	12089	"BIGDB	84	13	0	0	96	0	72	95
2.	95*	1120214	7705	"BIGDB	77	19	0	0	96	4	72	93
3.	86	112403	12729	"BIGDB	85	12	2	0	81	4	60	31
4.	86	629505	12223	"BIGDB	84	24	2	0	89	2	60	31
5.	83*	6975980	12689	"BIGDB	51	52	2	0	89	3	57	25

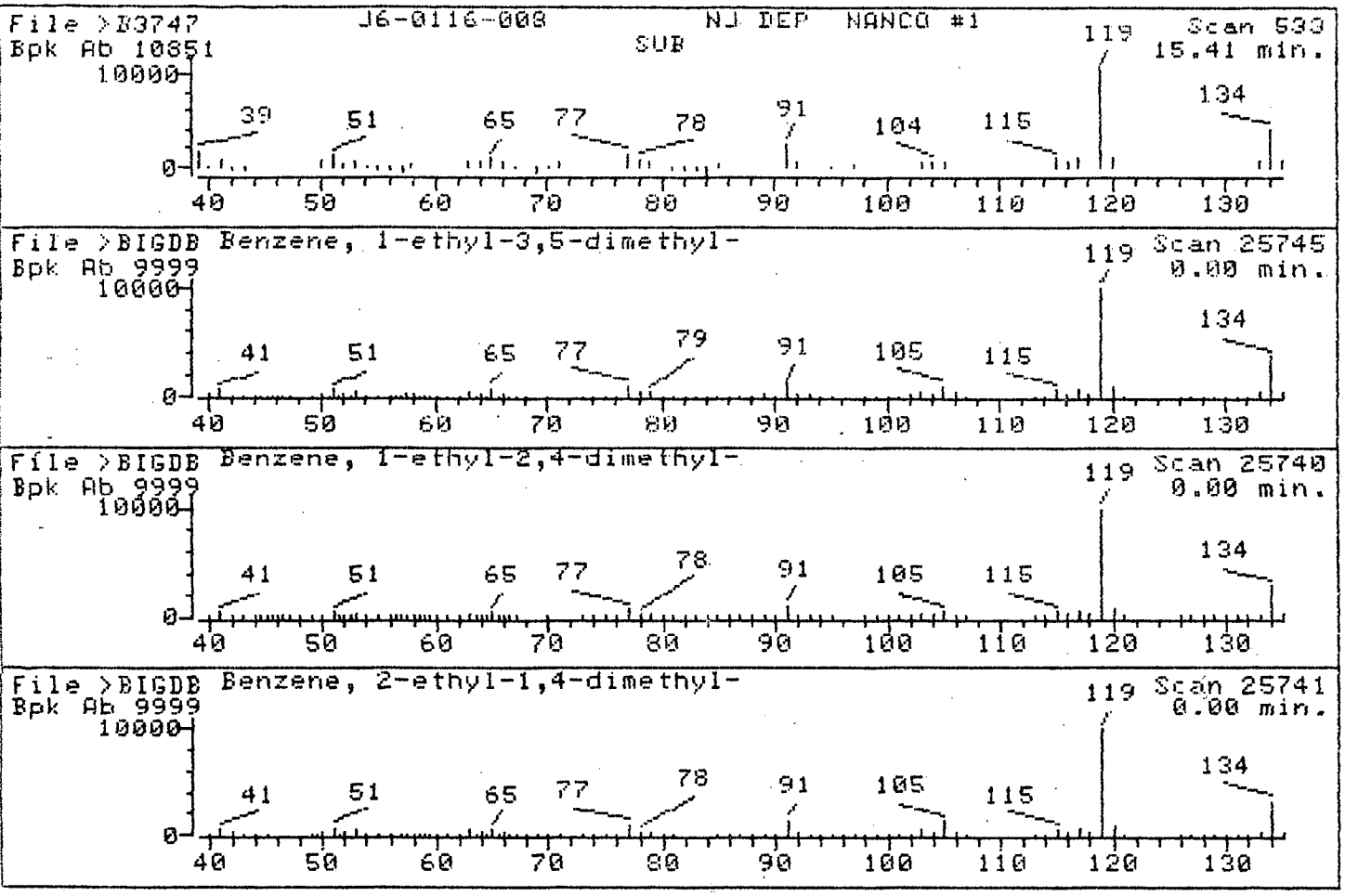


000238

1.	Benzene, 1,2,4,5-tetramethyl-	134 C10H14
2.	Benzene, 1-ethyl-3,5-dimethyl-	134 C10H14
3.	Benzene, 1-methyl-4-(1-methylethyl)-	134 C10H14
4.	Benzene, 1-ethyl-3,5-dimethyl-	134 C10H14
5.	Benzene, 1-ethyl-2,3-dimethyl-	134 C10H14

Sample file: >B3747 Spectrum #: 528
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	87*	95932	25739	"BIGDB	67	35	0	0	78	13	55	80
2.	84*	934747	25745	"BIGDB	65	31	1	0	100	8	55	65
3.	83*	99876	26158	"BIGDB	62	30	0	0	100	13	51	74
4.	83*	934747	26176	"BIGDB	58	31	0	0	100	12	51	71
5.	83*	933982	26173	"BIGDB	59	35	1	0	100	9	54	53

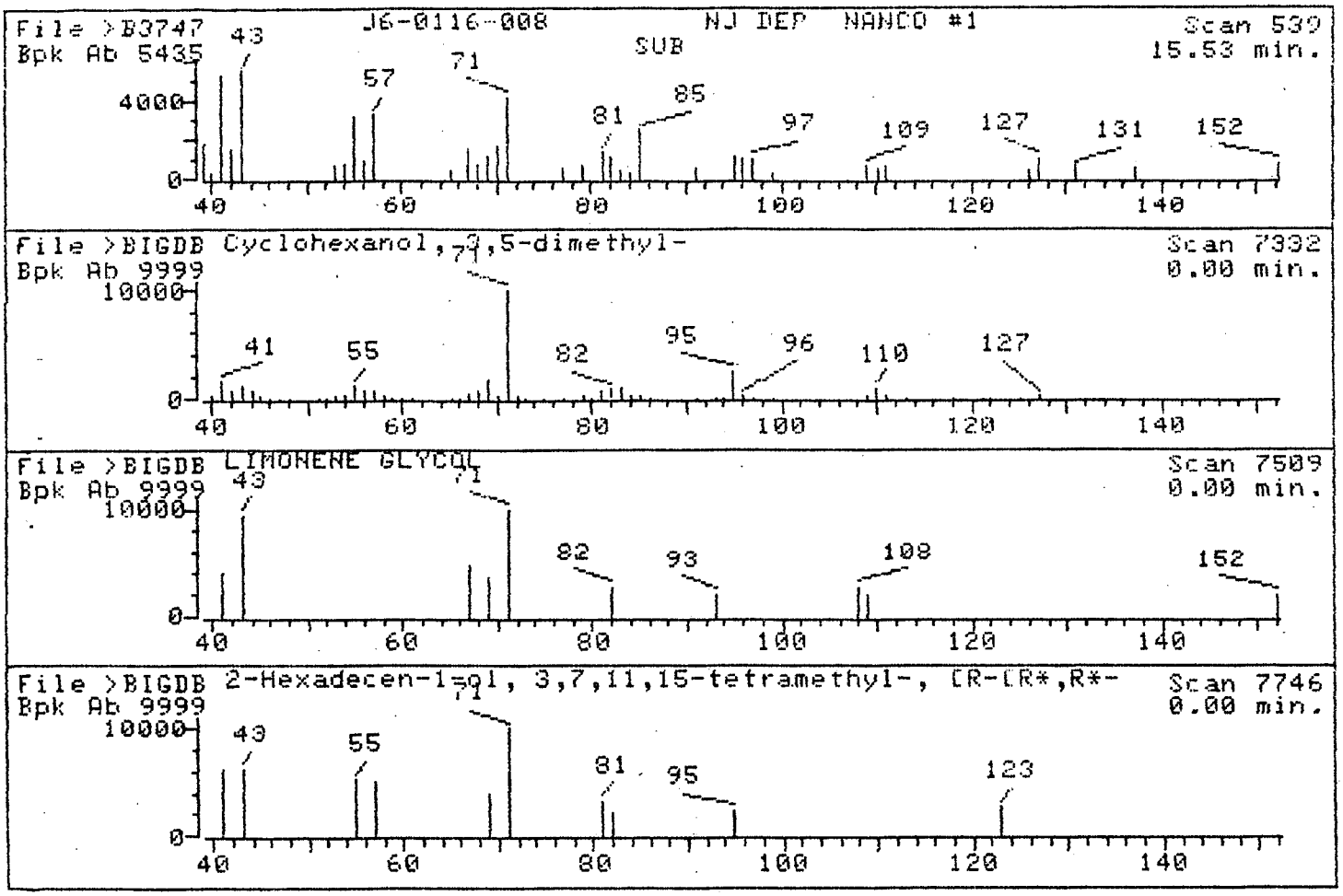


000239

1.	Benzene, 1-ethyl-3,5-dimethyl-	134 C10H14
2.	Benzene, 1-ethyl-2,4-dimethyl-	134 C10H14
3.	Benzene, 2-ethyl-1,4-dimethyl-	134 C10H14
4.	Benzene, 2-ethyl-1,3-dimethyl-	134 C10H14
5.	Benzene, 1-methyl-3-(1-methylethyl)-	134 C10H14

Sample file: >B3747 Spectrum #: 533
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	88*	934747	25745	"BIGDB	70	26	2	0	92	0	65	54
2.	86*	874419	25740	"BIGDB	52	37	2	0	100	3	60	35
3.	86*	1758889	25741	"BIGDB	53	41	2	0	89	5	60	34
4.	86*	2870044	25742	"BIGDB	50	38	2	0	100	1	60	31
5.	86*	535773	25737	"BIGDB	50	39	2	0	100	5	60	31

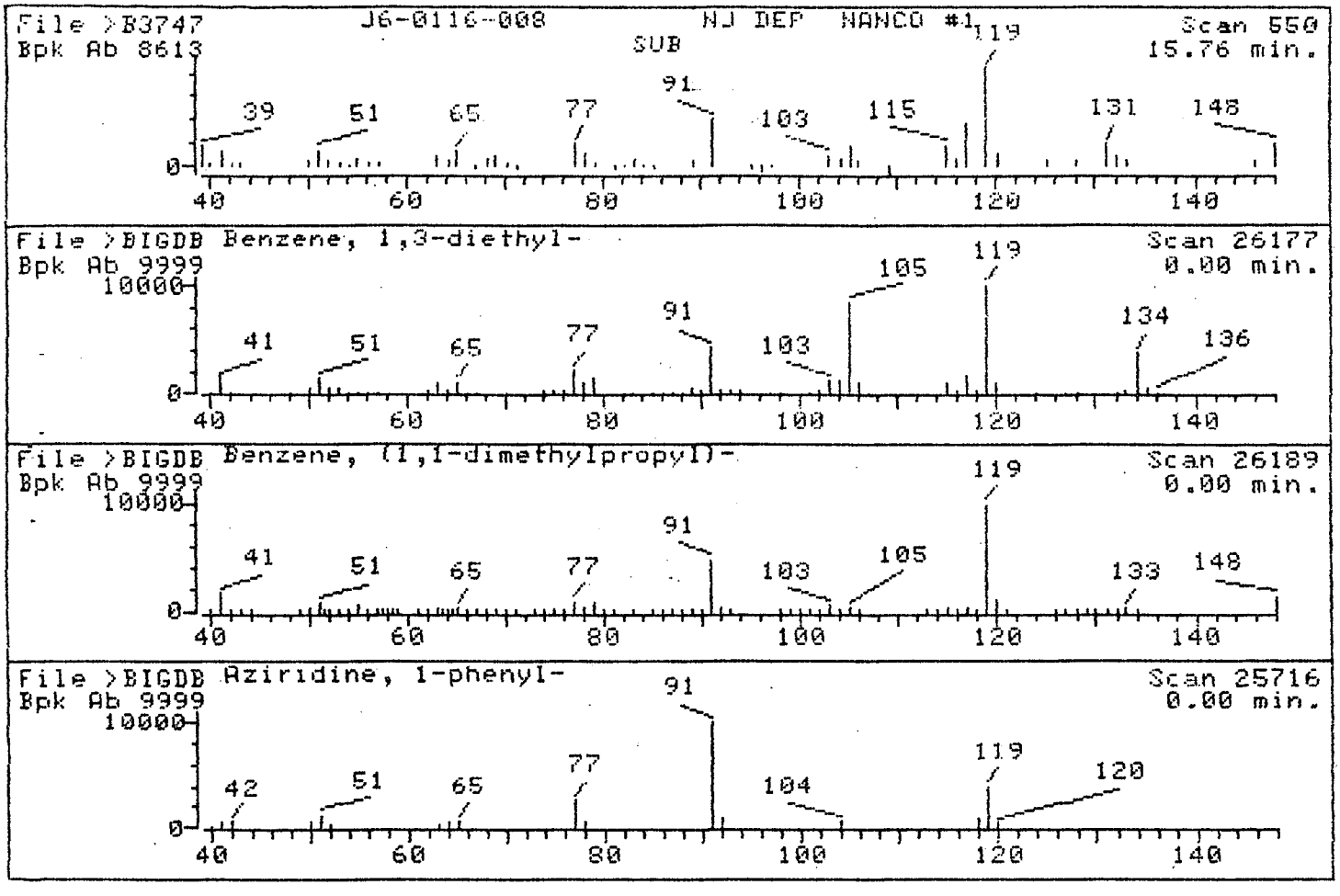


000240

1.	Cyclohexanol, 3,5-dimethyl-	128	C8H16O
2.	LIMONENE GLYCOL	196	C12H20O2
3.	2-Hexadecen-1-ol, 3,7,11,15-tetramethyl-, [R-[R*,R*-(E)]]-	296	C20H40O
4.	1-Hexene, 3,4,5-trimethyl-	126	C9H18
5.	TRIMETHYL-2,4,4 HEXENE-1	126	C9H18

Sample file: >B3747 Spectrum #: 539
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	20	5441521	7332	"BIGDB	33	54	1	0	75	51	5	12
2.	20	0	7509	"BIGDB	48	30	2	0	59	54	5	16
3.	20	150867	7746	"BIGDB	37	35	2	0	75	54	5	12
4.	11*	56728100	7321	"BIGDB	32	53	2	0	100	63	2	16
5.	11*	0	7322	"BIGDB	27	64	3	0	75	62	2	13

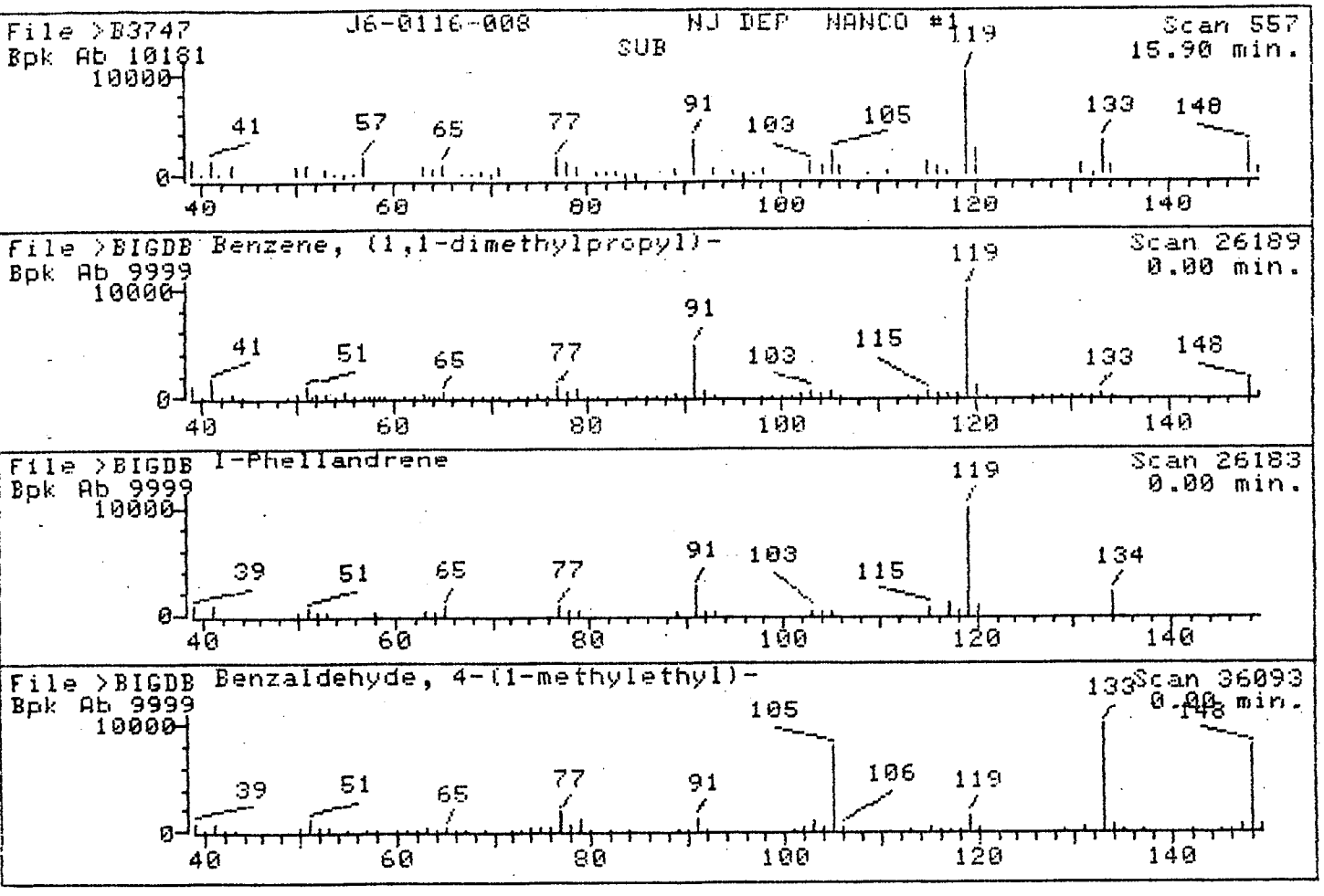


000241

1. Benzene, 1,3-diethyl-	134	C10H14
2. Benzene, (1,1-dimethylpropyl)-	148	C11H16
3. Aziridine, 1-phenyl-	119	C8H9N
4. Cyclohexene, 3-methylene-4-(1,2-propadienyl)-	132	C10H12
5. Benzene, isocyanato-	119	C7H5NO

Sample file: >B3747 Spectrum #: 550
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	25	141935	26177	"BIGDB	62	48	2	0	91	48	7	13
2.	20*	2049958	26189	"BIGDB	28	62	2	0	96	55	5	14
3.	15*	696184	25716	"BIGDB	24	68	3	0	249	56	3	12
4.	13*	68377811	25080	"BIGDB	57	50	2	0	43	64	3	34
5.	11*	103719	26140	"BIGDB	34	49	2	0	100	64	2	17

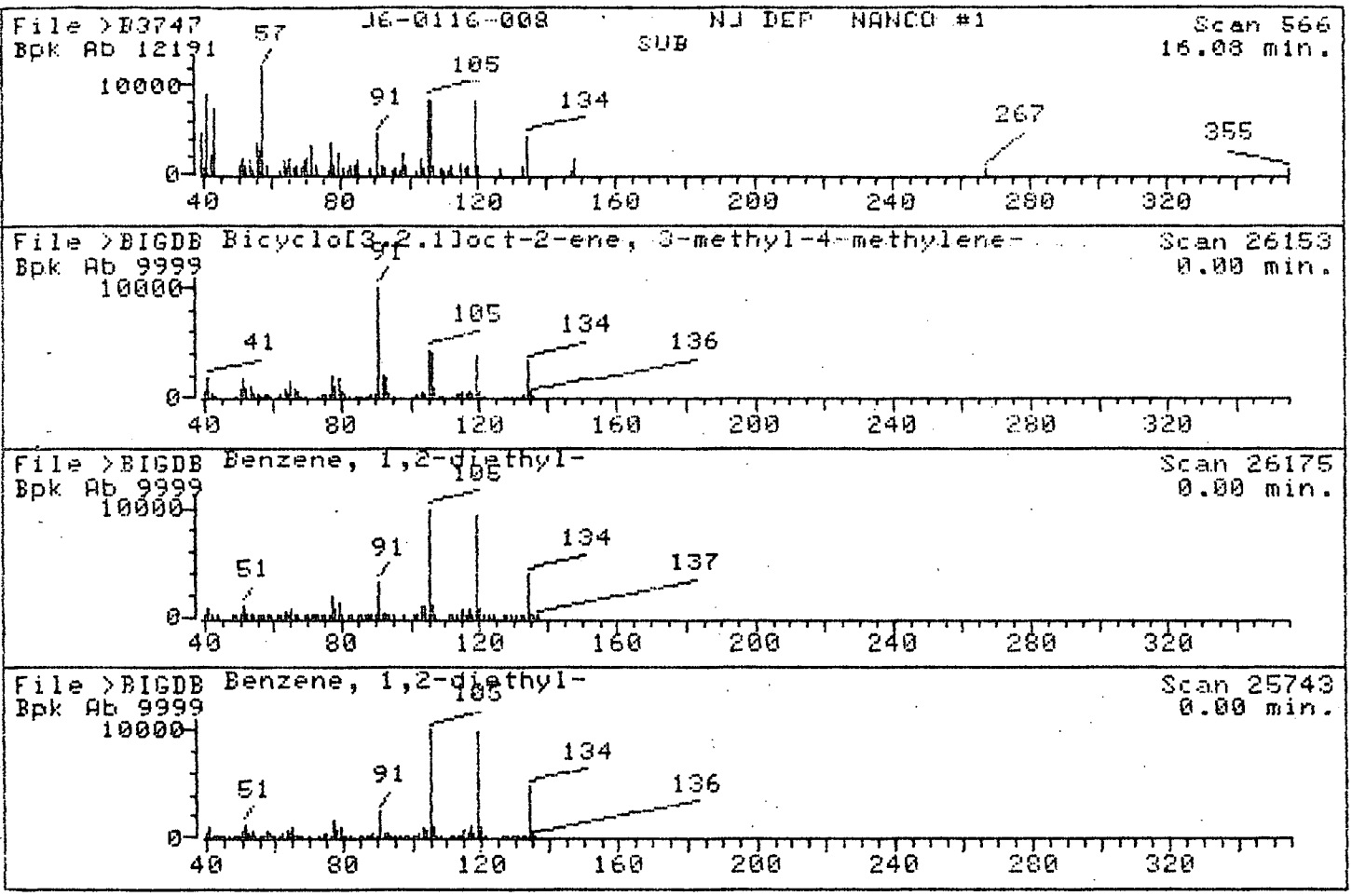


000242

1. Benzene, (1,1-dimethylpropyl)-	148	C11H16
2. 1-Phellandrene	136	C10H16
3. Benzaldehyde, 4-(1-methylethyl)-	148	C10H12O
4. Benzene, isocyanato-	119	C7H5NO
5. IMIDAZO[1,5-A]PYRIDINE	119	C6H5N3

Sample file: >B3747 Spectrum #: 557
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	25*	2049958	26189	"BIGDB	20	70	2	0	70	47	7	13
2.	20	99832	26183	"BIGDB	45	38	2	0	100	51	5	15
3.	15*	122032	36093	"BIGDB	29	59	1	0	27	60	3	16
4.	15*	103719	26140	"BIGDB	22	61	3	0	100	56	3	12
5.	15*	0	25710	"BIGDB	22	68	3	0	100	58	3	12

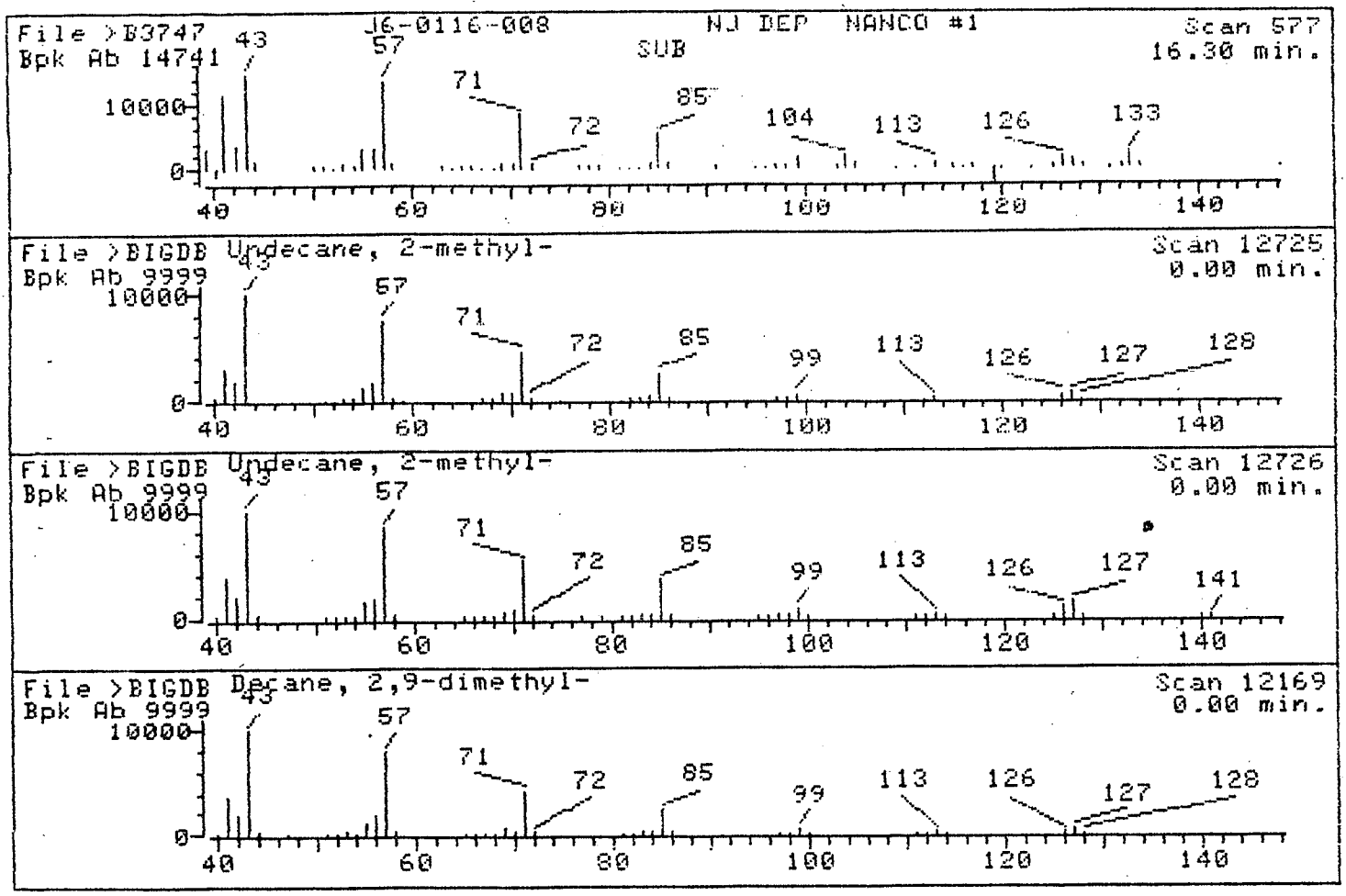


000243

1.	Bicyclo[3.2.1]oct-2-ene, 3-methyl-4-methylene-	134 C10H14
2.	Benzene, 1,2-diethyl-	134 C10H14
3.	Benzene, 1,2-diethyl-	134 C10H14
4.	Benzene, 1,3-diethyl-	134 C10H14
5.	Benzene, 1,3-diethyl-	134 C10H14

Sample file: >B3747 Spectrum #: 566
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	31*	49826531	26153	"BIGDB	26	83	2	0	106	35	12	14
2.	31*	135013	26175	"BIGDB	63	42	1	0	69	56	8	60
3.	31*	135013	25743	"BIGDB	57	49	0	0	62	58	8	69
4.	31*	141935	25746	"BIGDB	51	51	0	0	62	58	8	61
5.	23*	141935	26177	"BIGDB	63	47	2	0	69	56	6	41

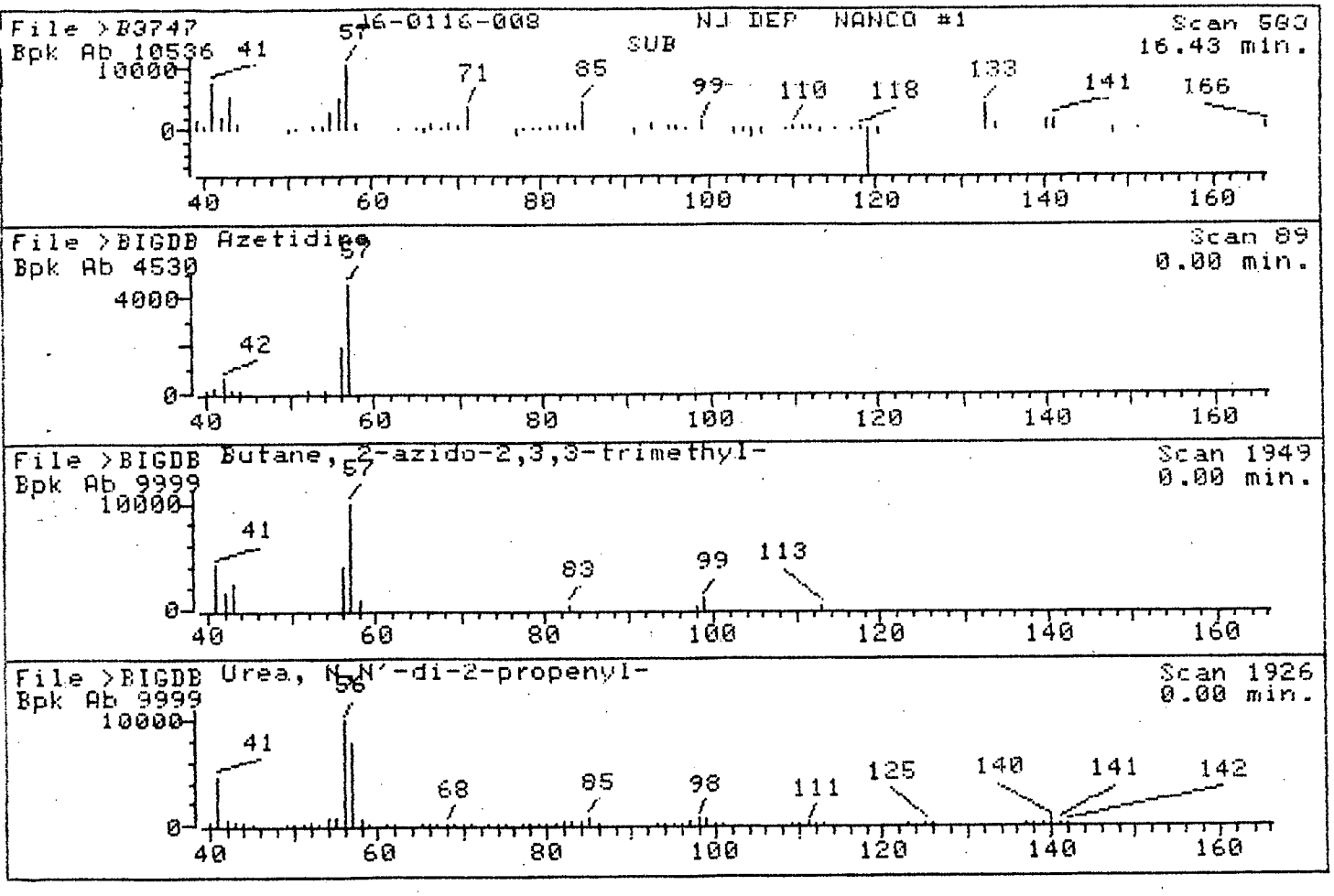


000244

1.	Undecane, 2-methyl-	170 C12H26
2.	Undecane, 2-methyl-	170 C12H26
3.	Decane, 2,9-dimethyl-	170 C12H26
4.	Dodecane, 2,6,11-trimethyl-	212 C15H32
5.	Undecane, 2-methyl-	170 C12H26

Sample file: >B3747 Spectrum #: 577
Search speed: 1 Tilting option: N No. of ion ranges searched: 47

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	67	7045718	12725	"BIGDB	67	27	2	0	100	11	34	23
2.	67	7045718	12726	"BIGDB	71	33	2	0	91	11	34	25
3.	67	1002171	12169	"BIGDB	60	32	2	0	100	14	34	21
4.	60	31295564	7738	"BIGDB	61	63	2	0	68	15	30	12
5.	60	7045718	12167	"BIGDB	61	38	2	0	100	11	30	19

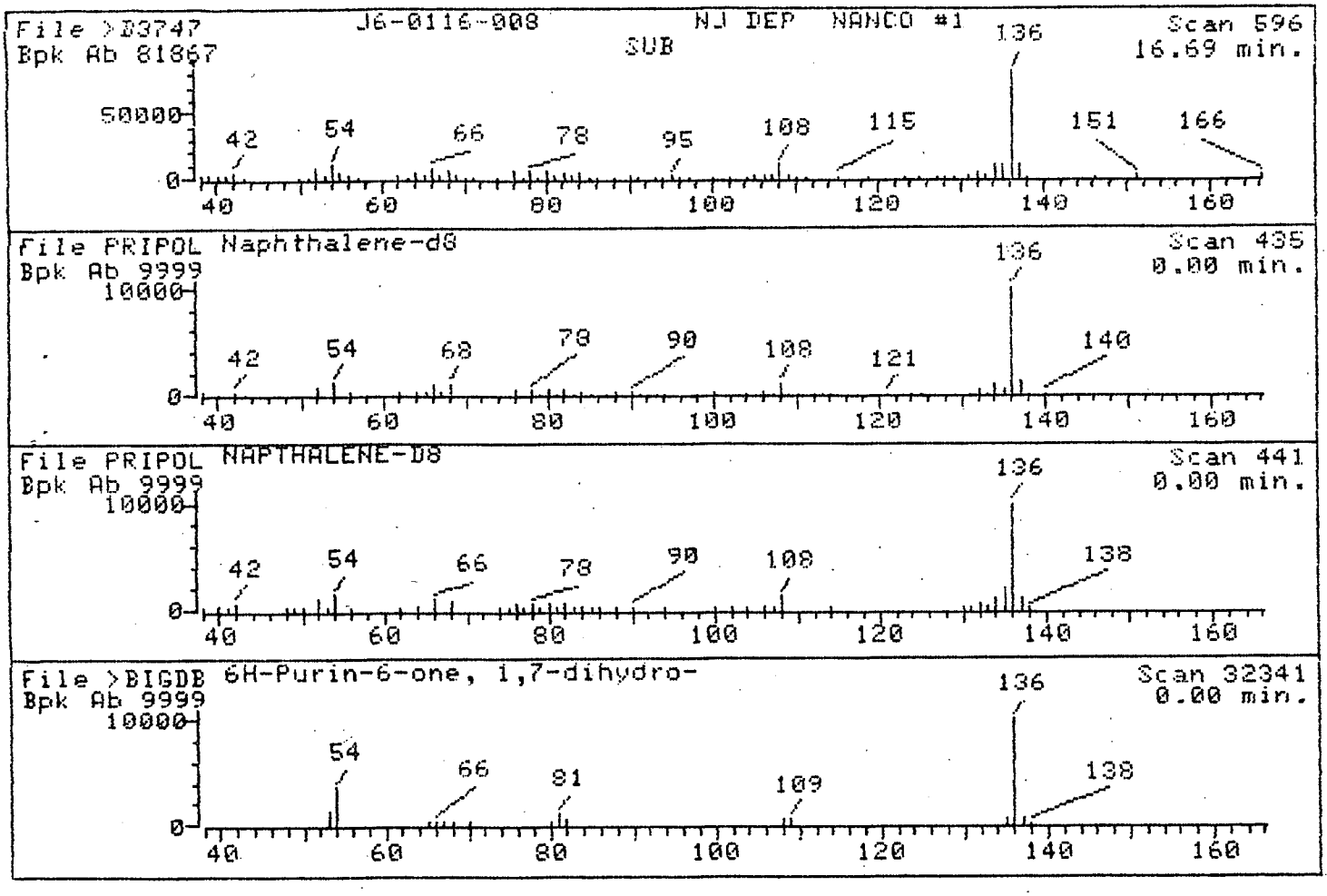


000245

1. Azetidine — 57 C3H7N
2. Butane, 2-azido-2,3,3-trimethyl- — 141 C7H15N3
3. Urea, N,N'-di-2-propenyl- — 140 C7H12N2O

Sample file: >B3747 Spectrum #: 583
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	25*	503297	89	"BIGDB	23	64	1	0	141	50	7	14
2.	25	51677419	1949	"BIGDB	38	27	2	0	94	45	8	13
3.	15*	1801725	1926	"BIGDB	26	64	3	0	130	56	3	13



000246

1. Naphthalene-d8 — 136 C10.D8

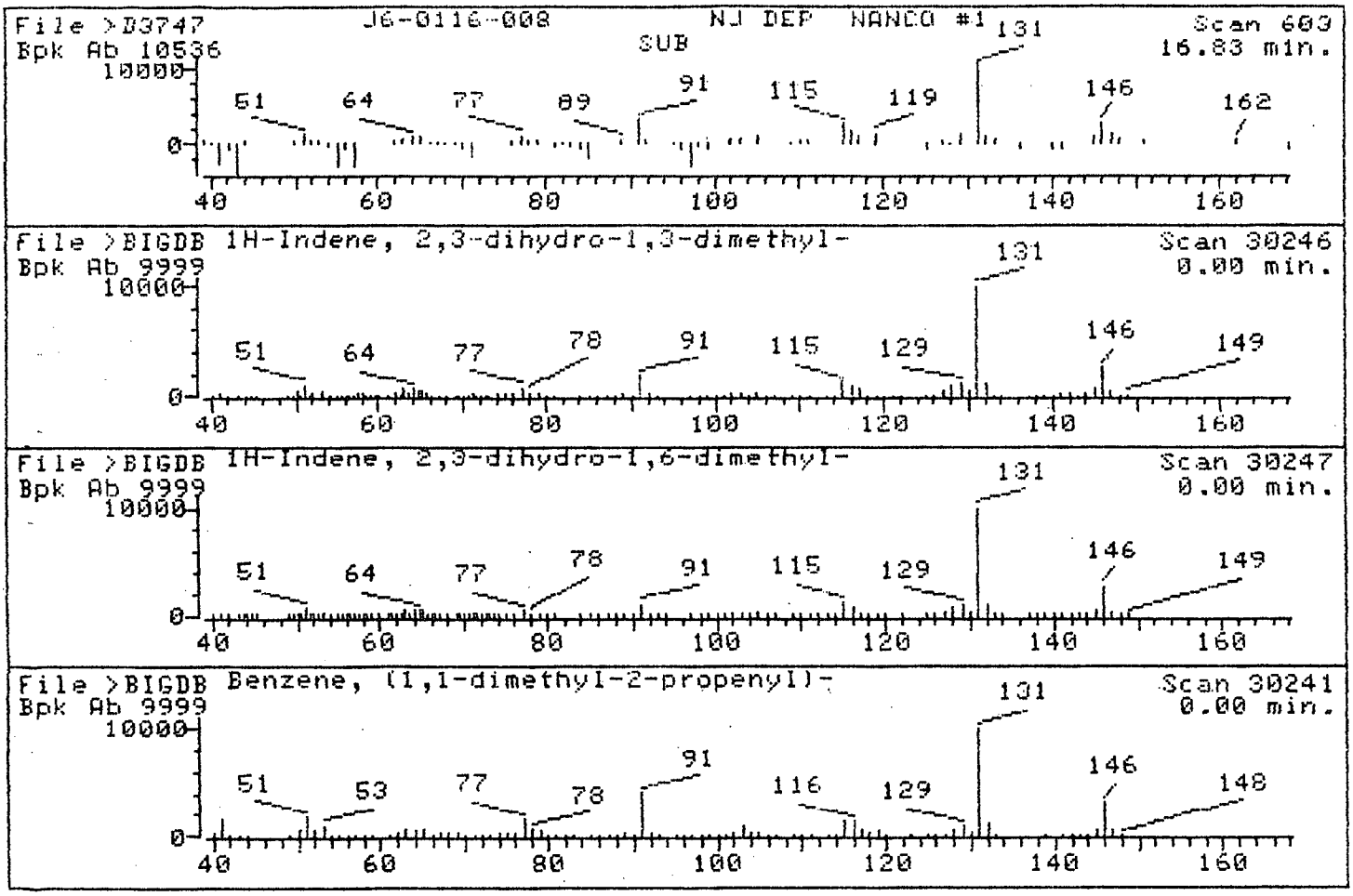
2. NAPTHALENE-D8 — 136 C10.D8.

INTERNAL STD. — BNA

3. 6H-Purin-6-one, 1,7-dihydro- — 136 C5H4N4O
4. 7H-Pyrazolo[4,3-d]pyrimidin-7-one, 1,4-dihydro- — 136 C5H4N4O
5. 2,1,3-Benzothiadiazole — 136 C6H4N2S

Sample file: >B3747 Spectrum #: 596
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	94*	435	208	PRIPOL	80	13	1	0	100	6	68	93
2.	75*	441	209	PRIPOL	75	27	1	0	61	30	37	73
3.	44*	68940	32341	"BIGDB	38	47	3	0	100	25	17	15

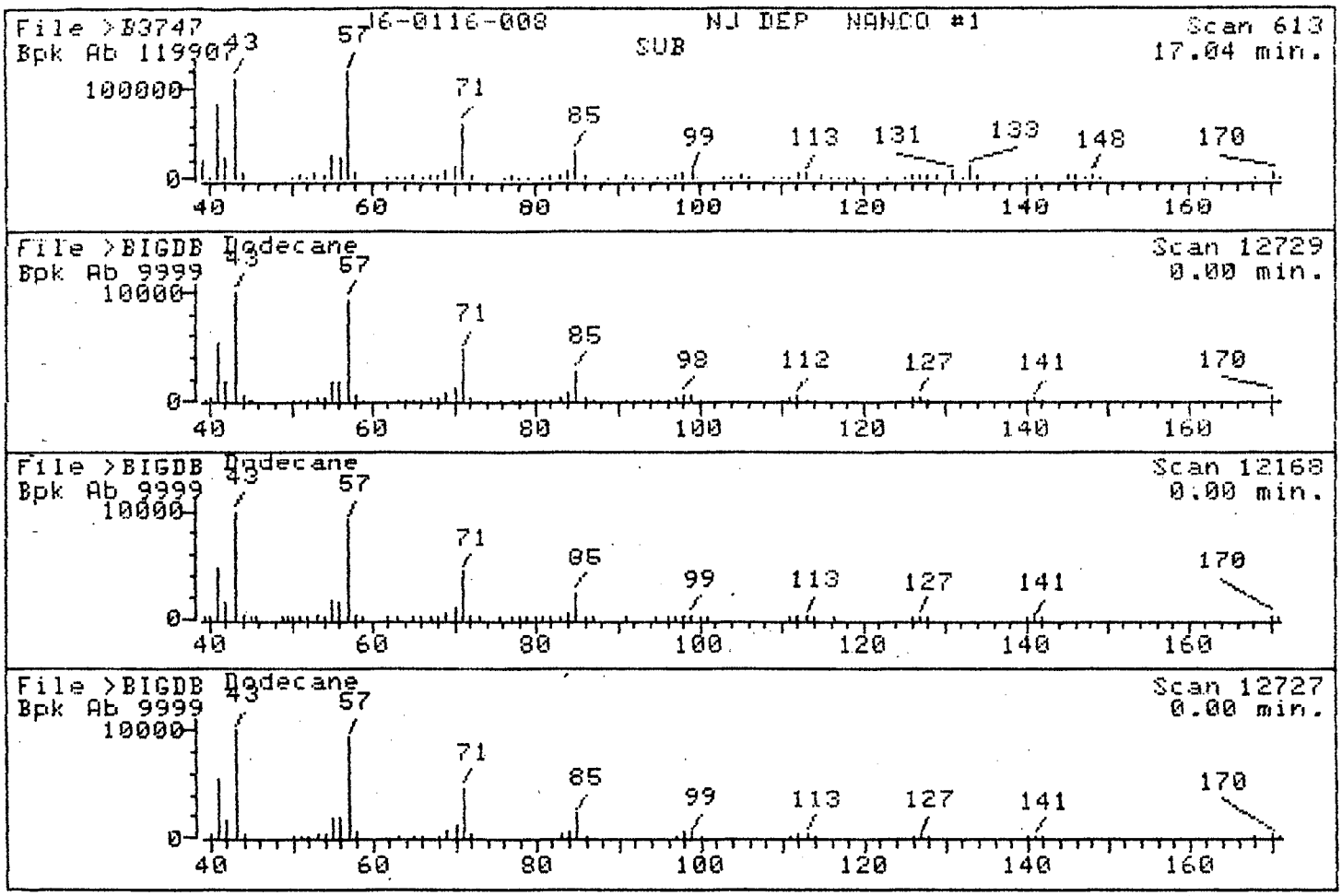


000247

1.	1H-Indene, 2,3-dihydro-1,3-dimethyl-	146 C11H14
2.	1H-Indene, 2,3-dihydro-1,6-dimethyl-	146 C11H14
3.	Benzene, (1,1-dimethyl-2-propenyl)-	146 C11H14
4.	1H-Indene, 2,3-dihydro-1,1-dimethyl-	146 C11H14
5.	1,1-DIMETHYL-2-PHENYLCYCLOPROPANE	146 C11H14

Sample file: >B3747 Spectrum #: 603
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	74*	4175535	30246	"BIGDB	69	33	2	0	91	14	39	49
2.	63*	17059482	30247	"BIGDB	57	43	2	0	94	19	30	34
3.	58*	18321363	30241	"BIGDB	50	52	2	0	80	18	25	23
4.	42*	4912929	30244	"BIGDB	40	53	2	0	98	28	14	19
5.	35*	0	30254	"BIGDB	34	17	0	0	49	50	11	33

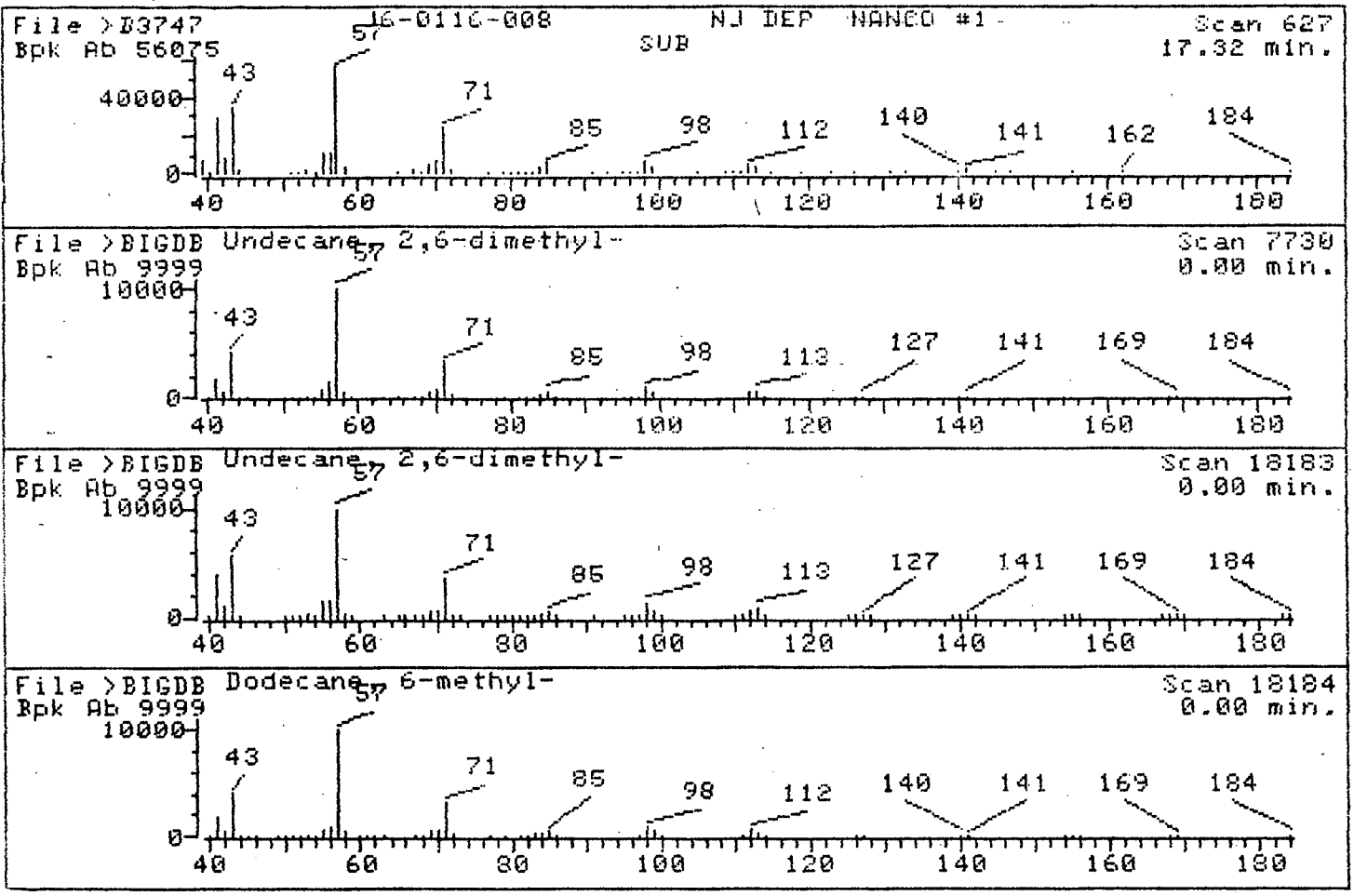


000248

1. Dodecane	170	C12H26
2. Dodecane	170	C12H26
3. Dodecane	170	C12H26
4. Dodecane	170	C12H26
5. Tridecane	184	C13H28

Sample file: >B3747 Spectrum #: 613
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	97*	112403	12729	"BIGDB	97	0	0	0	90	10	68	97
2.	95*	112403	12168	"BIGDB	91	8	0	0	93	12	64	96
3.	94*	112403	12727	"BIGDB	79	18	0	0	93	11	64	94
4.	86*	112403	12728	"BIGDB	59	34	0	0	97	10	59	72
5.	83	629505	12750	"BIGDB	87	20	1	0	81	10	54	50



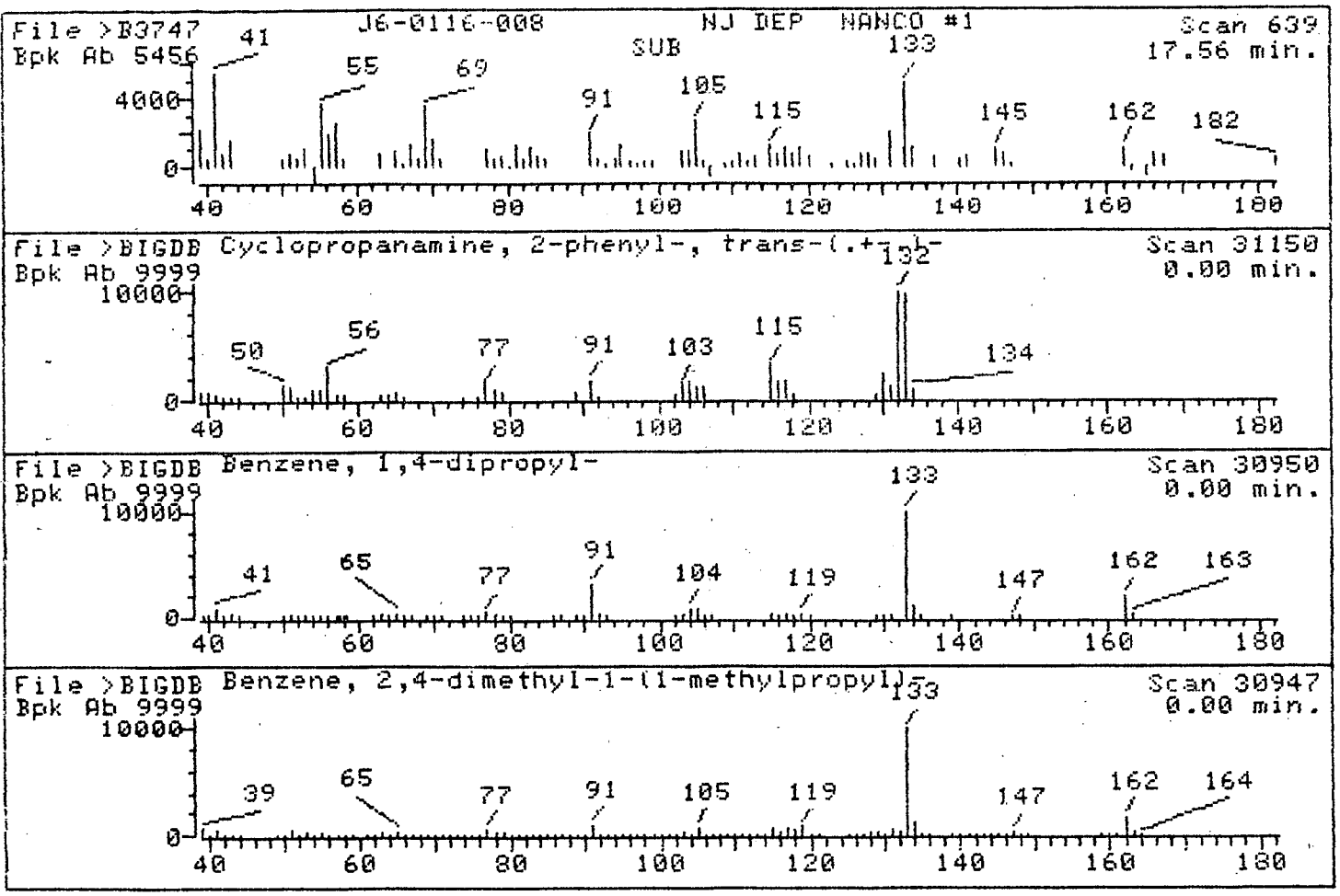
000249

1. Undecane, 2,6-dimethyl- 184 C13H28
2. Undecane, 2,6-dimethyl- 184 C13H28
3. Dodecane, 6-methyl- 184 C13H28
4. Undecane, 3,6-dimethyl- 184 C13H28
5. Decane, 2,6,8-trimethyl- 184 C13H28

Hyd

Sample file: >B3747 Spectrum #: 627
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	95*	17301234	7730	"BIGDB	76	19	0	0	100	0	72	93
2.	88*	17301234	18183	"BIGDB	74	28	2	0	86	0	65	56
3.	86*	6044719	18184	"BIGDB	64	33	0	0	97	8	59	77
4.	83*	17301289	7486	"BIGDB	61	37	1	0	86	6	54	57
5.	79*	62108263	7482	"BIGDB	51	41	2	0	100	8	48	33

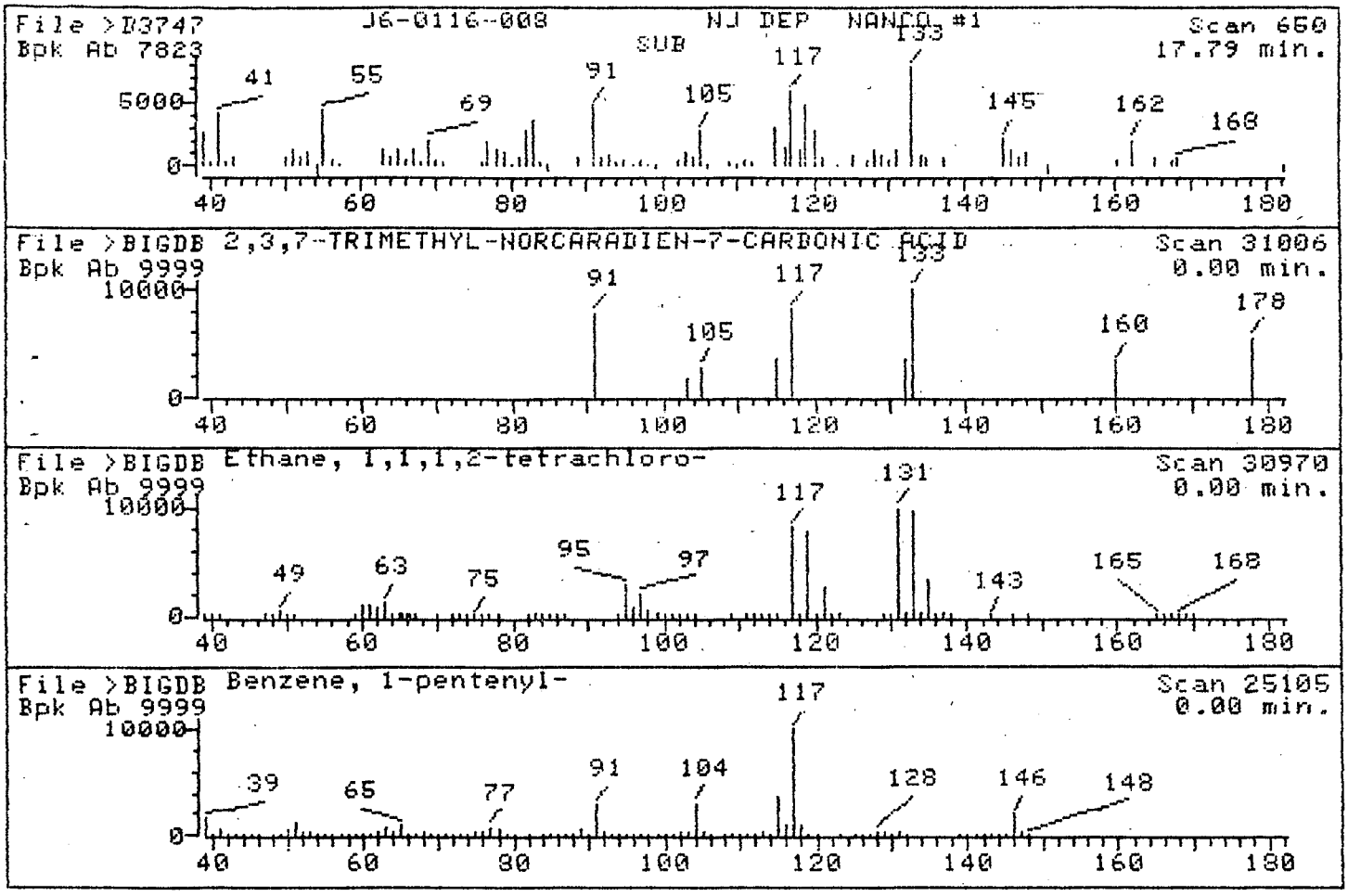


000250

1. Cyclopropanamine, 2-phenyl-, trans-(.+-.)- 133 C9H11N
2. Benzene, 1,4-dipropyl- 162 C12H18
3. Benzene, 2,4-dimethyl-1-(1-methylpropyl)- 162 C12H18
4. 6H,7H,8H-2-PYRINDINE, 3-METHYL- 133 C9H11N
5. Quinoline, 1,2,3,4-tetrahydro- 133 C9H11N

Sample file: >B3747 Spectrum #: 639
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	28*	155099	31150	"BIGDB	56	62	2	0	86	54	8	33
2.	25*	4815570	30950	"BIGDB	29	63	2	0	88	50	7	14
3.	25*	1483609	30947	"BIGDB	21	71	2	0	88	47	7	13
4.	20*	0	30881	"BIGDB	30	67	2	0	85	53	5	14
5.	20*	635461	31149	"BIGDB	29	79	3	0	107	53	5	13

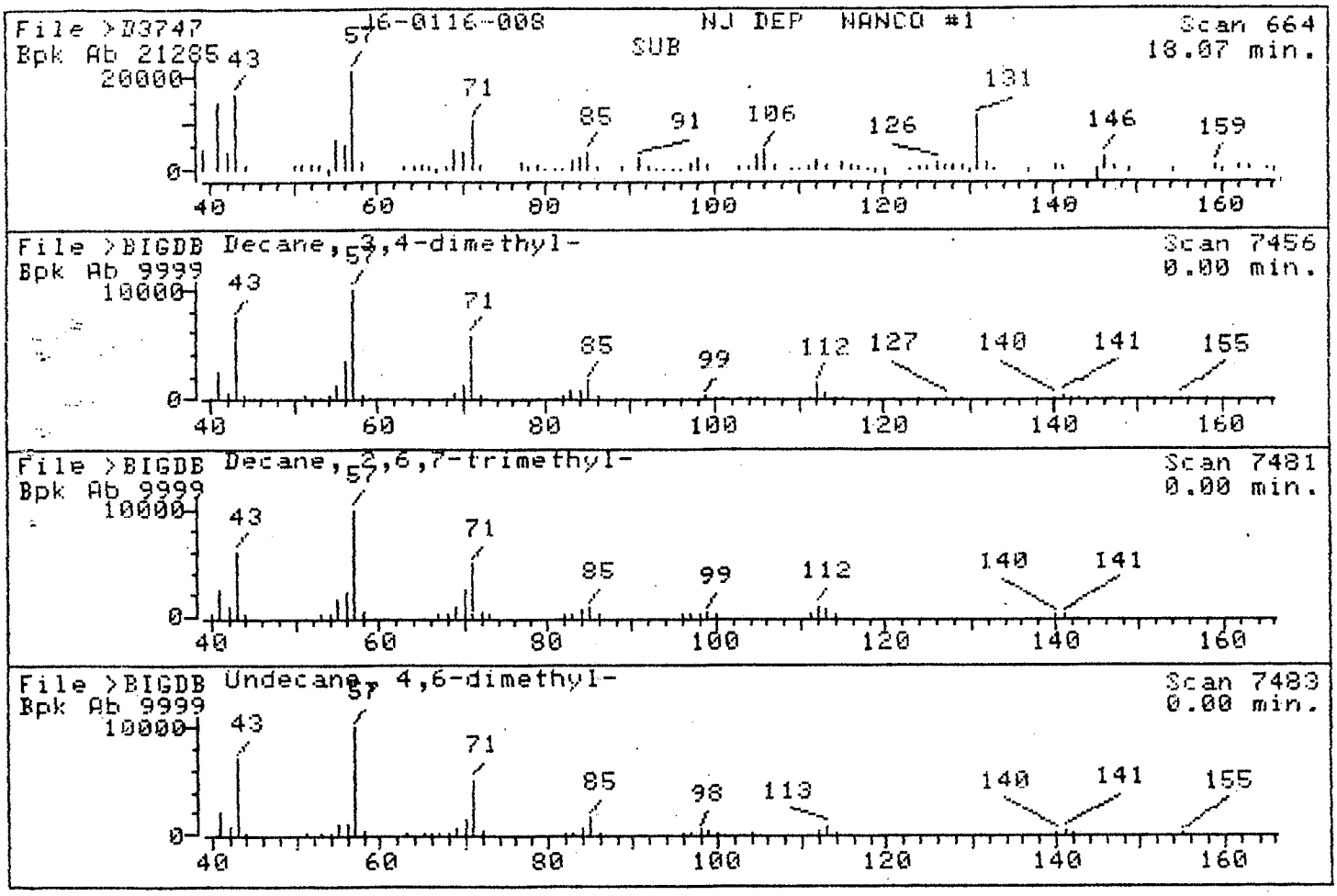


000251

1. 2,3,7-TRIMETHYL-NORCARADIEN-7-CARBONIC ACID 178 C11H14O2
2. Ethane, 1,1,1,2-tetrachloro- 166 C2H2Cl4
3. Benzene, 1-pentenyl- 146 C11H14
4. Benzene, (1-ethyl-2-propenyl)- 146 C11H14
5. 2-T-BUTYL-3,7-DEHYDROTROPONE 160 C11H12O

Sample file: >B3747 Spectrum #: 650
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	26	0	31006	"BIGDB	43	36	2	0	76	44	8	14
2.	25*	630206	30970	"BIGDB	30	91	3	0	76	44	8	13
3.	11*	826186	25105	"BIGDB	38	63	2	0	74	63	2	14
4.	11*	19947229	25104	"BIGDB	30	59	2	0	74	63	2	15
5.	11	0	25131	"BIGDB	65	56	2	0	59	65	2	14

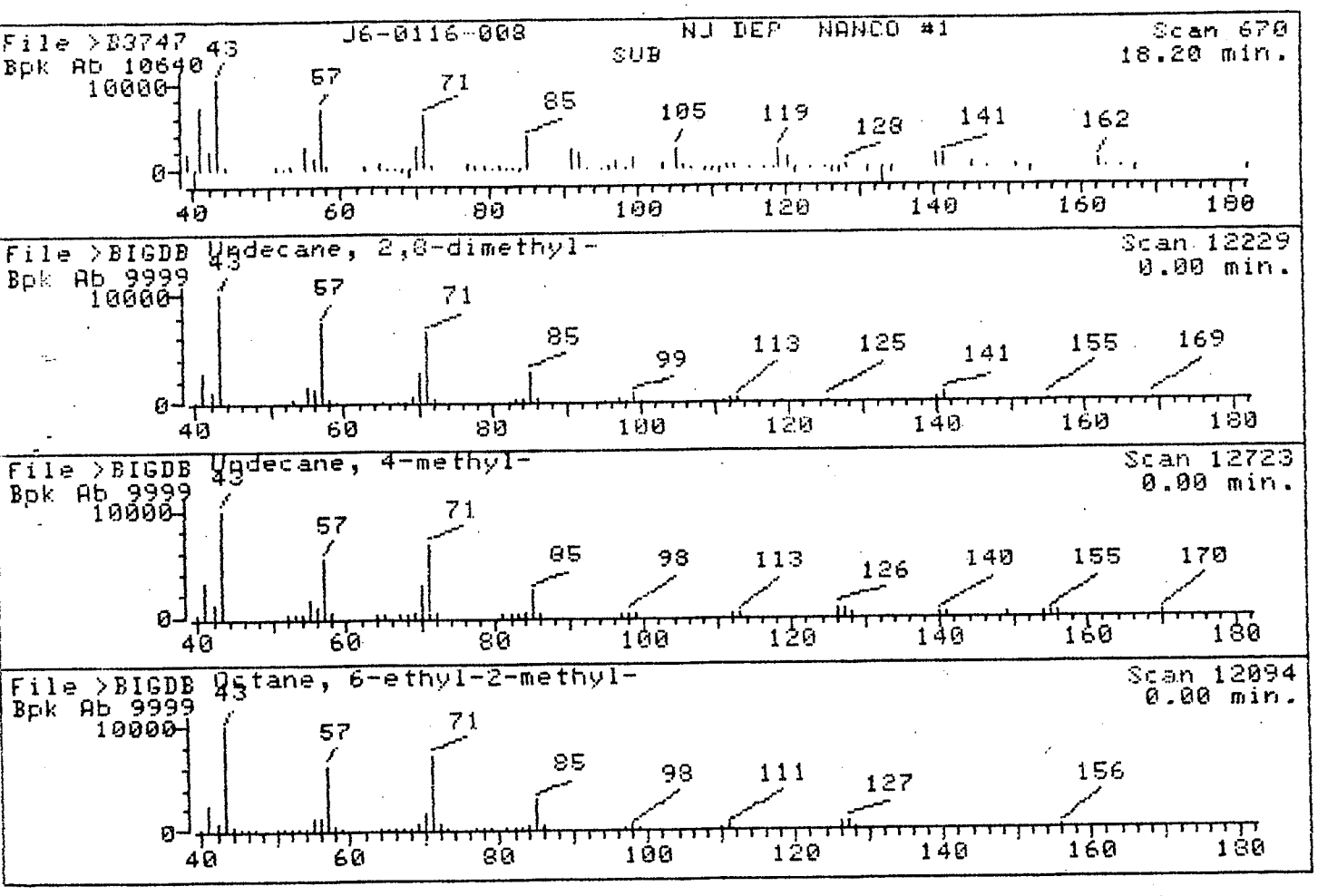


000252

1. Decane, 3,4-dimethyl-	170	C12H26
2. Decane, 2,6,7-trimethyl-	184	C13H28
3. Undecane, 4,6-dimethyl-	184	C13H28
4. Nonane, 3-methyl-	142	C10H22
5. Butane, 2,2-dimethyl-	86	C6H14

Sample file: >B3747 Spectrum #: 664
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	56	17312457	7456	"BIGDB	73	21	1	0	74	29	24	36
2.	37	62108252	7481	"BIGDB	54	44	2	0	99	30	14	14
3.	32	17312822	7483	"BIGDB	55	43	2	0	96	34	12	15
4.	32	5911046	7679	"BIGDB	44	42	1	0	81	35	12	15
5.	31	75832	7616	"BIGDB	40	51	0	0	68	41	12	22

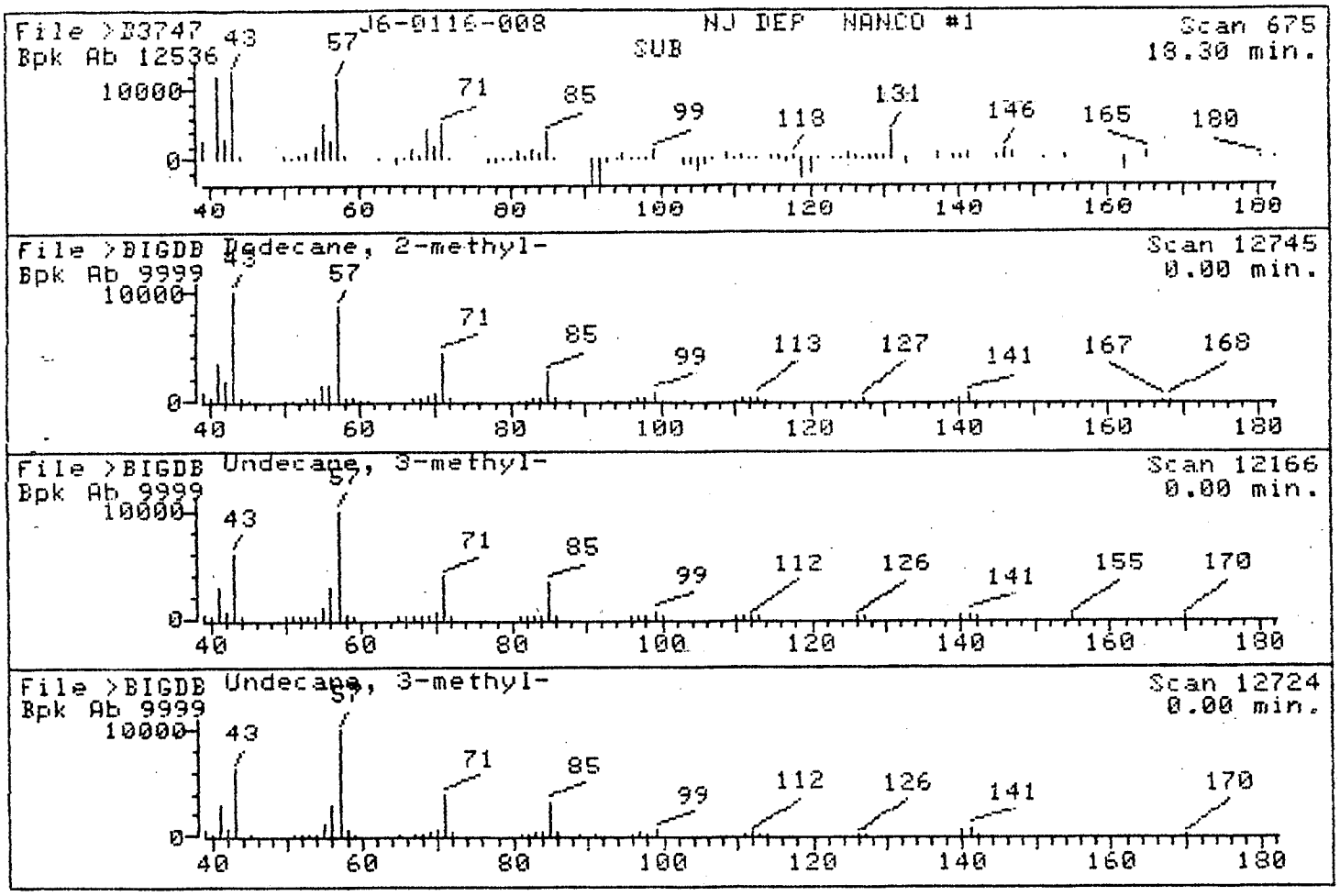


000253

1. Undecane, 2,8-dimethyl- 184 C13H28
2. Undecane, 4-methyl- 170 C12H26
3. Octane, 6-ethyl-2-methyl- 156 C11H24

Sample file: >B3747 Spectrum #: 670
Search speed: 1 Tilting option: N No. of ion ranges searched: 49

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	20	17301256	12229	"BIGDB	60	44	2	0	86	53	5	14
2.	15	2980690	12723	"BIGDB	45	49	2	0	80	59	3	12
3.	11	62016197	12094	"BIGDB	41	49	2	0	82	62	2	12

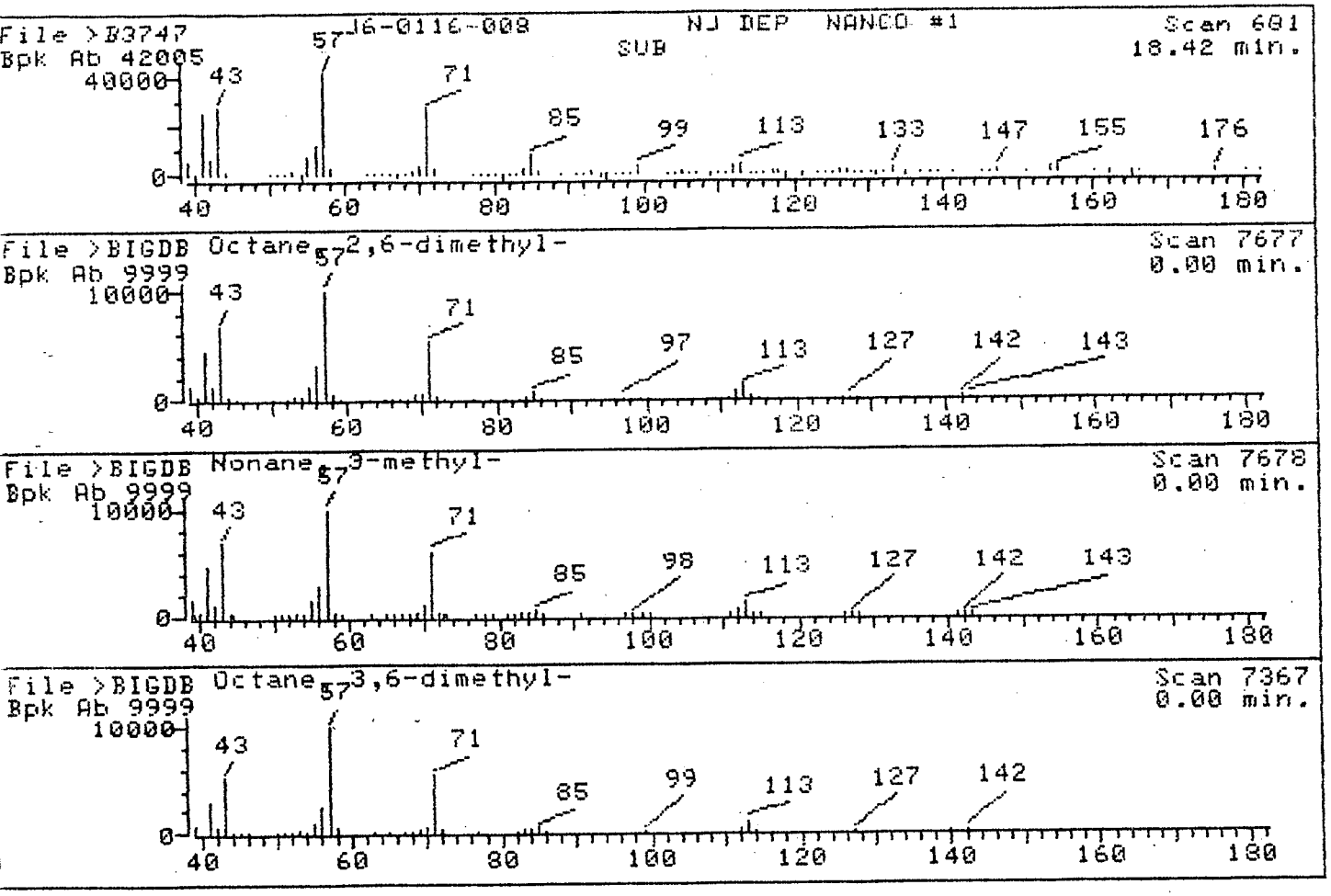


000254

1.	Dodecane, 2-methyl-	184 C13H28
2.	Undecane, 3-methyl-	170 C12H26
3.	Undecane, 3-methyl-	170 C12H26
4.	Undecane	156 C11H24
5.	Decane, 2,9-dimethyl-	170 C12H26

Sample file: >B3747 Spectrum #: 675
Search speed: 1 Tilting option: N No. of ion ranges searched: 46

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	55	1560970	12745	"BIGDB	72	29	1	0	95	26	24	35
2.	53	1002433	12166	"BIGDB	68	20	1	0	74	28	24	33
3.	53	1002433	12724	"BIGDB	68	23	1	0	71	28	24	33
4.	52	1120214	12089	"BIGDB	59	38	3	0	107	19	20	13
5.	52	1002171	12169	"BIGDB	54	38	2	0	97	19	20	19

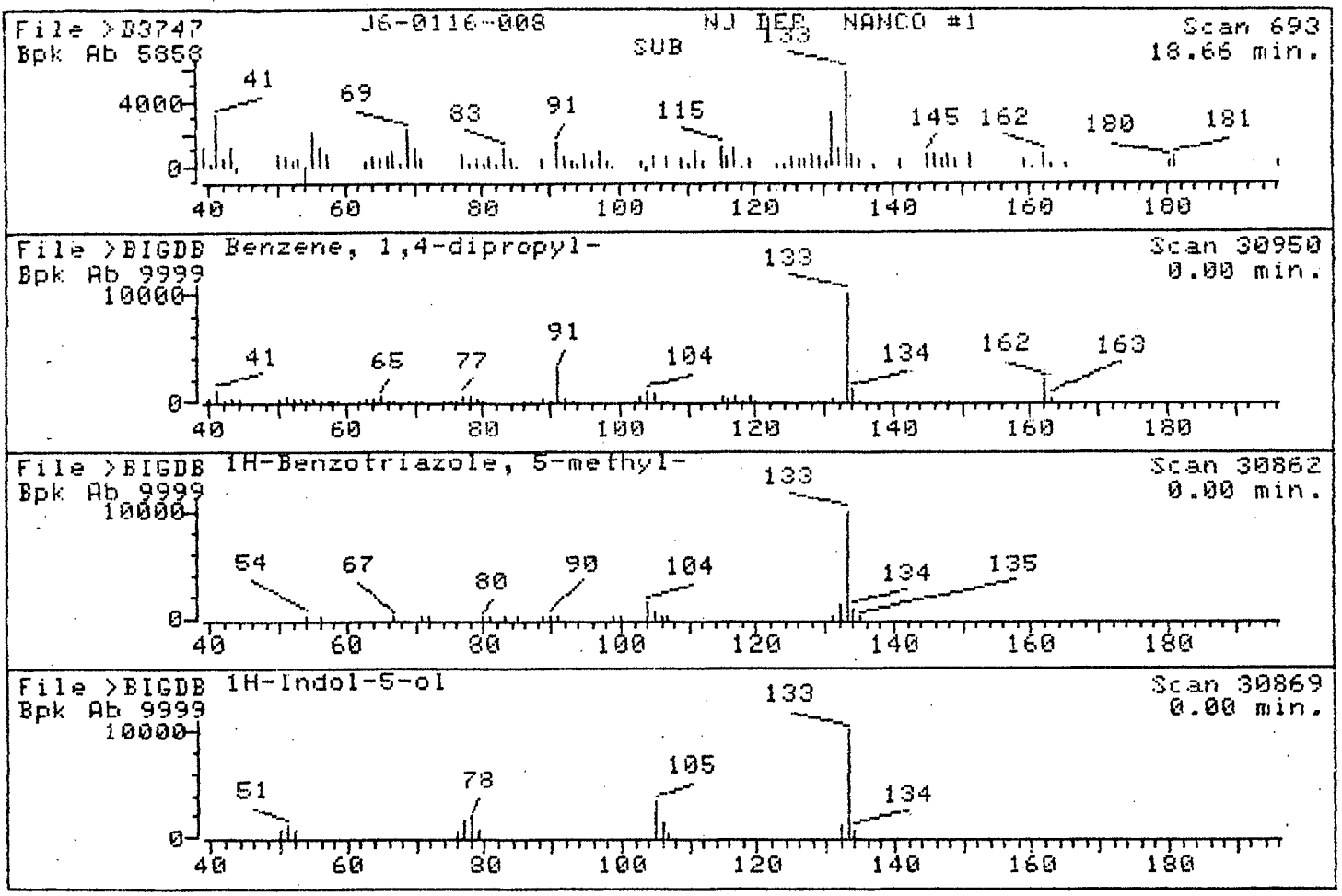


000255

1.	Octane, 2,6-dimethyl-	142 C10H22
2.	Nonane, 3-methyl-	142 C10H22
3.	Octane, 3,6-dimethyl-	142 C10H22
4.	Nonane, 3-methyl-	142 C10H22
5.	Nonane, 3-methyl-	142 C10H22

Sample file: >B3747 Spectrum #: 681
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	71	2051301	7677	"BIGDB	68	24	1	0	85	13	38	33
2.	71	5911046	7678	"BIGDB	70	27	1	0	69	13	38	35
3.	67	15869940	7367	"BIGDB	61	27	1	0	100	13	34	27
4.	63	5911046	7679	"BIGDB	65	21	1	0	100	16	30	31
5.	60	5911046	7680	"BIGDB	57	37	2	0	76	13	30	19

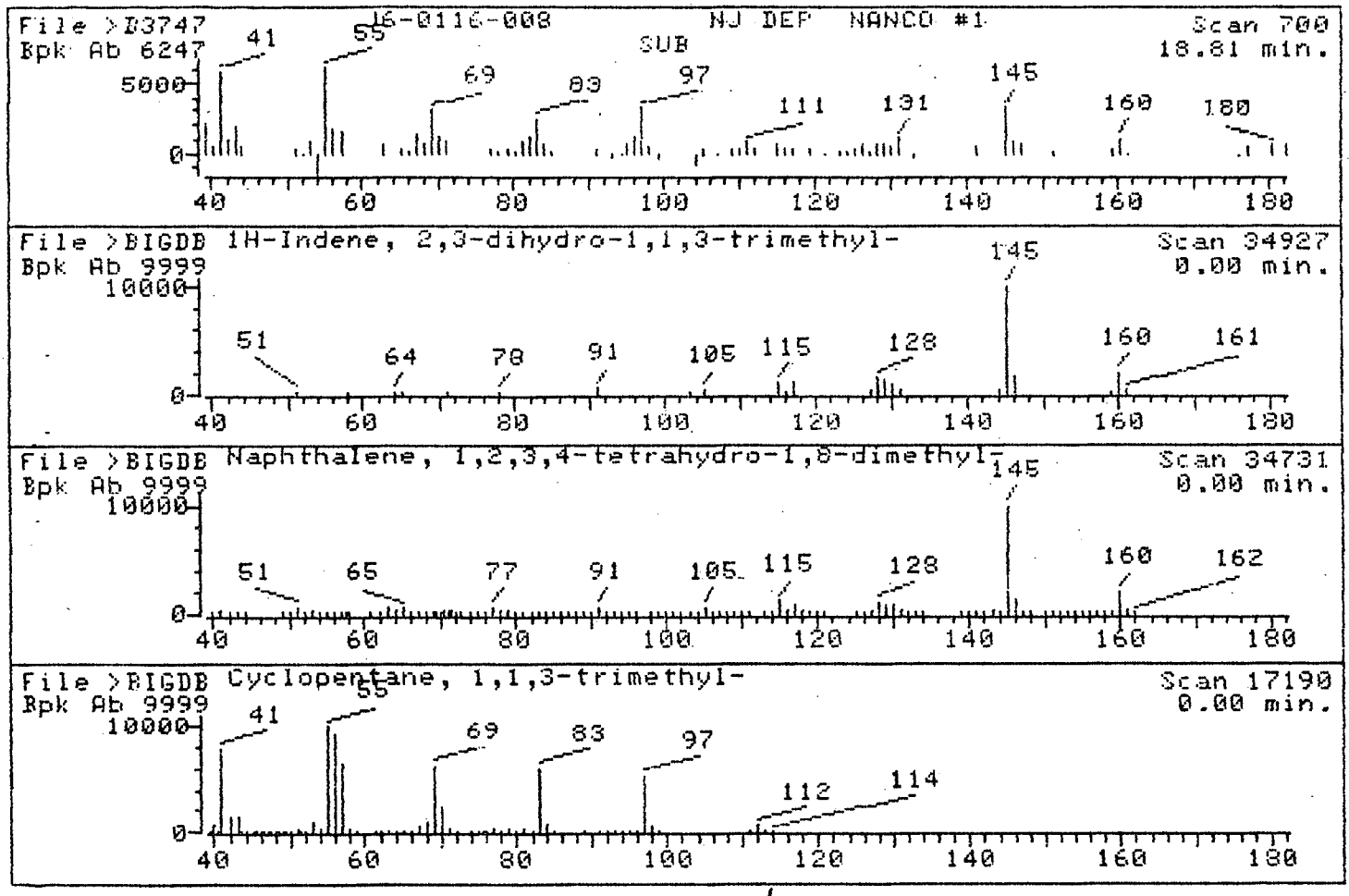


000256

1. Benzene, 1,4-dipropyl-	162	C12H18
2. 1H-Benzotriazole, 5-methyl-	133	C7H7N3
3. 1H-Indol-5-ol	133	C8H7NO
4. Benzene, 2,4-dimethyl-1-(1-methylpropyl)-	162	C12H18
5. M-TOLYL-DIMETHYLACETALDEHYDE	162	C11H14O

Sample file: >B3747 Spectrum #: 693
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	30*	4815570	30950	"BIGDB	41	51	1	0	68	47	10	23
2.	25*	136856	30862	"BIGDB	27	49	3	0	100	47	7	13
3.	25*	1953544	30869	"BIGDB	27	59	3	0	100	48	7	13
4.	25*	1483609	30947	"BIGDB	30	62	1	0	80	46	7	16
5.	25*	0	30944	"BIGDB	27	66	3	0	100	48	7	13



Unknown Poly Aromatic Hydr

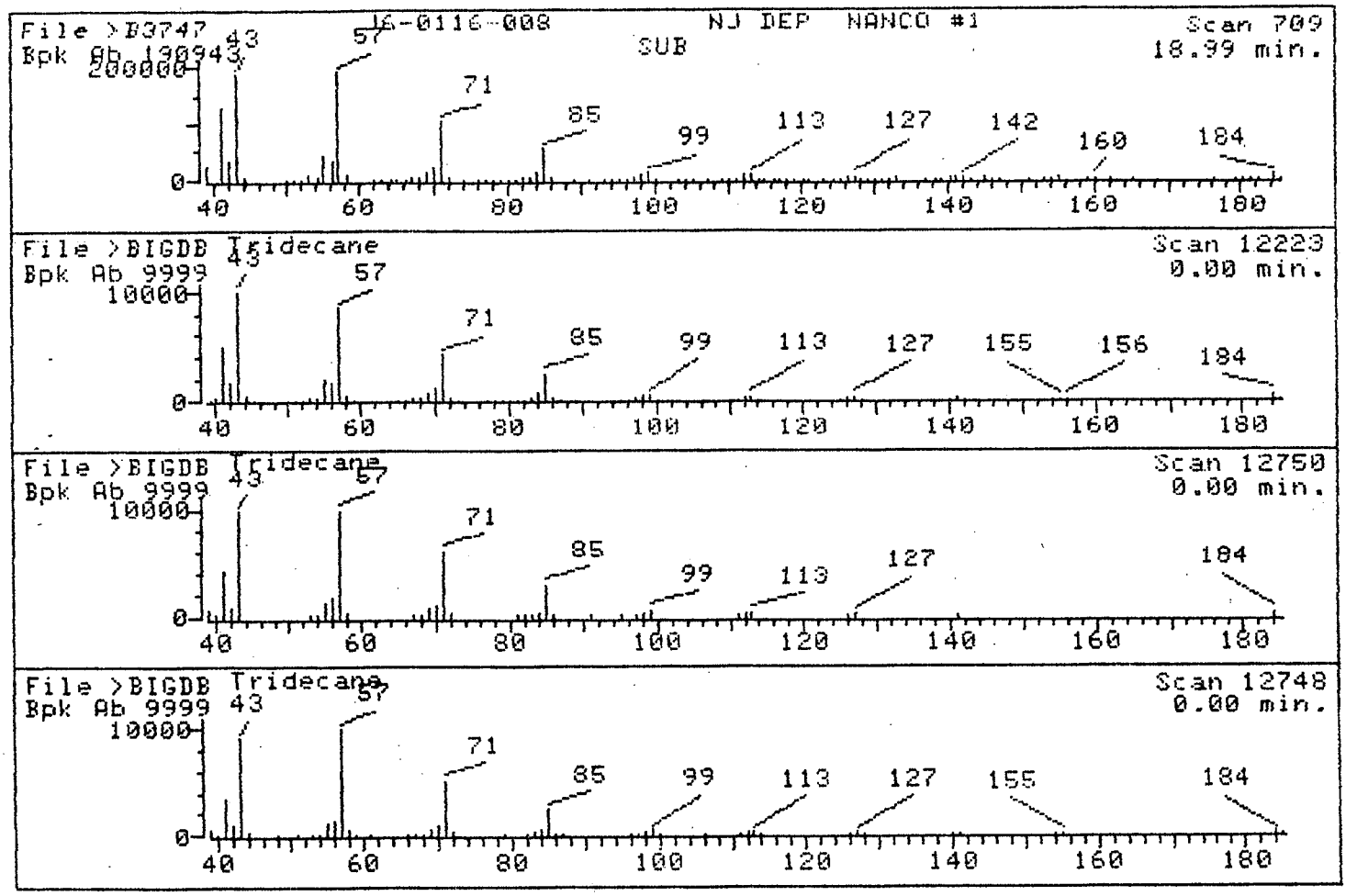
000257

/16

1. 1H-Indene, 2,3-dihydro-1,1,3-trimethyl- 160 C12H16
2. Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl- 160 C12H16
3. Cyclopentane, 1,1,3-trimethyl- 112 C8H16
4. Benzene, (1,3-dimethyl-2-butenyl)- 160 C12H16
5. Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)- 160 C12H16

Sample file: >B3747 Spectrum #: 700
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	21*	2613765	34927	"BIGDB	55	48	2	0	51	56	5	32
2.	18*	25419334	34731	"BIGDB	46	50	2	0	51	60	4	23
3.	18*	4516692	17190	"BIGDB	49	61	2	0	64	57	4	22
4.	15*	50704013	34733	"BIGDB	49	59	3	0	51	59	3	13
5.	15*	5557937	34713	"BIGDB	47	61	2	0	51	56	3	19

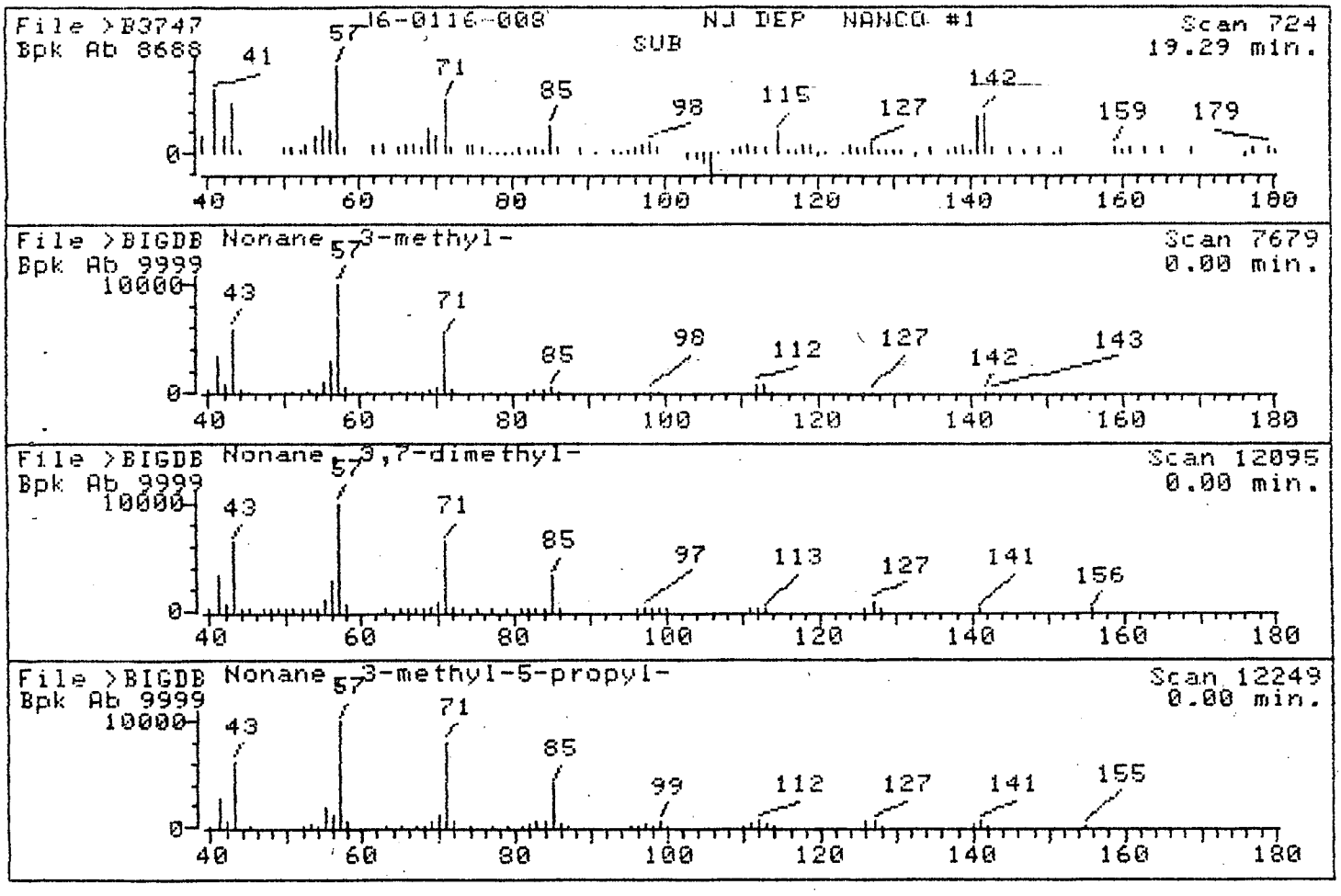


000258

1.	Tridecane	184 C13H28
2.	Tridecane	184 C13H28
3.	Tridecane	184 C13H28
4.	Dodecane	170 C12H26
5.	Hexadecane	226 C16H34

Sample file: >B3747 Spectrum #: 709
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	97*	629505	12223	"BIGDB	99	9	0	0	86	0	72	97
2.	95*	629505	12750	"BIGDB	94	13	1	0	81	0	72	93
3.	95*	629505	12748	"BIGDB	86	20	0	0	100	1	72	95
4.	89	112403	12729	"BIGDB	90	7	1	0	86	5	66	60
5.	87	544763	12354	"BIGDB	82	25	1	0	98	4	63	43

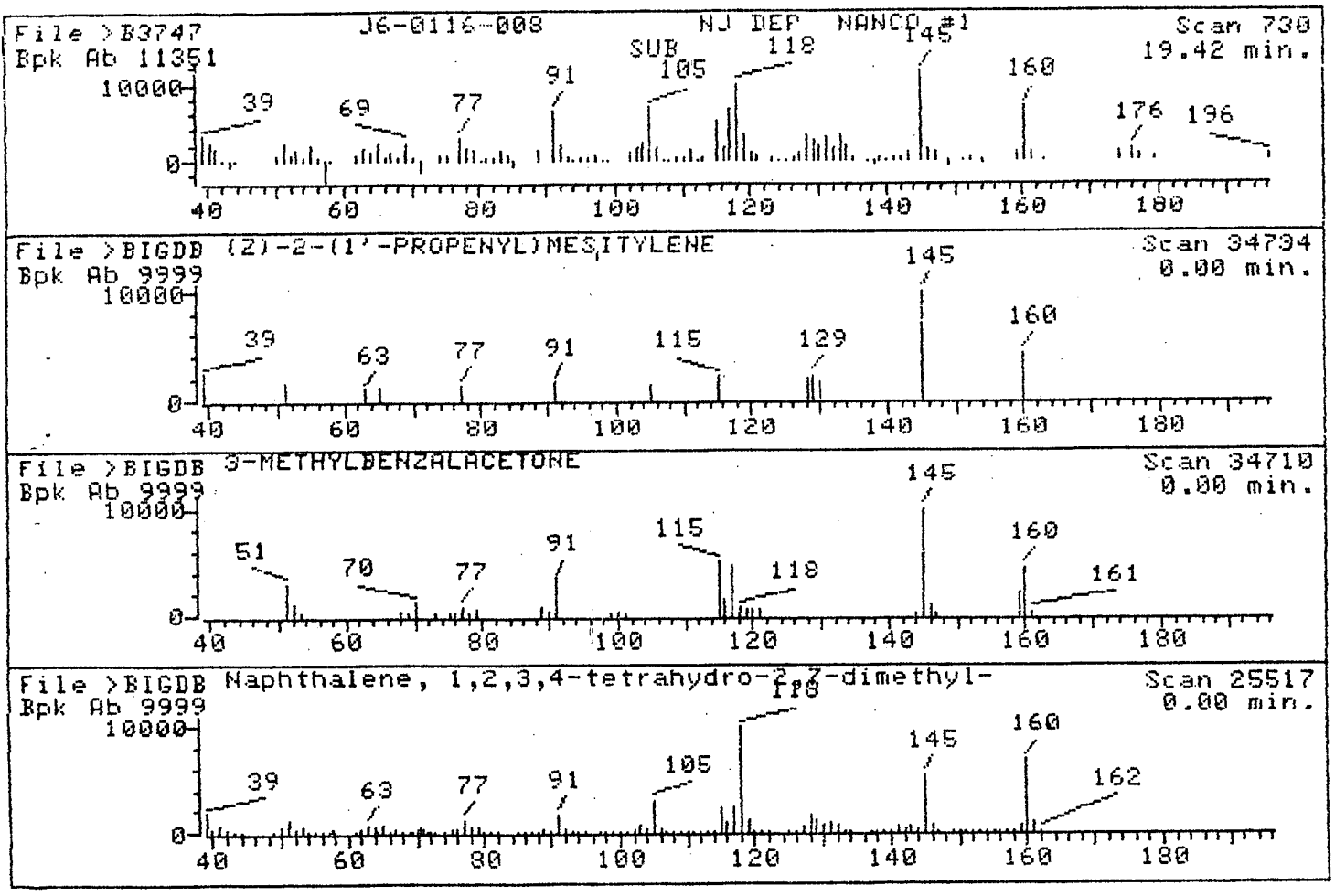


000259

1.	Nonane, 3-methyl-	142 C10H22
2.	Nonane, 3,7-dimethyl-	156 C11H24
3.	Nonane, 3-methyl-5-propyl-	184 C13H28
4.	Nonane, 3-methyl-	142 C10H22
5.	Nonane, 3-methyl-	142 C10H22

Sample file: >B3747 Spectrum #: 724
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	35*	5911046	7679	"BIGDB	49	37	1	0	80	49	11	37
2.	34	17302328	12095	"BIGDB	53	33	1	0	83	39	14	21
3.	32	31081182	12249	"BIGDB	66	39	1	0	73	42	12	23
4.	30*	5911046	7678	"BIGDB	46	51	2	0	80	47	10	22
5.	30*	5911046	7680	"BIGDB	44	50	2	0	74	48	10	23

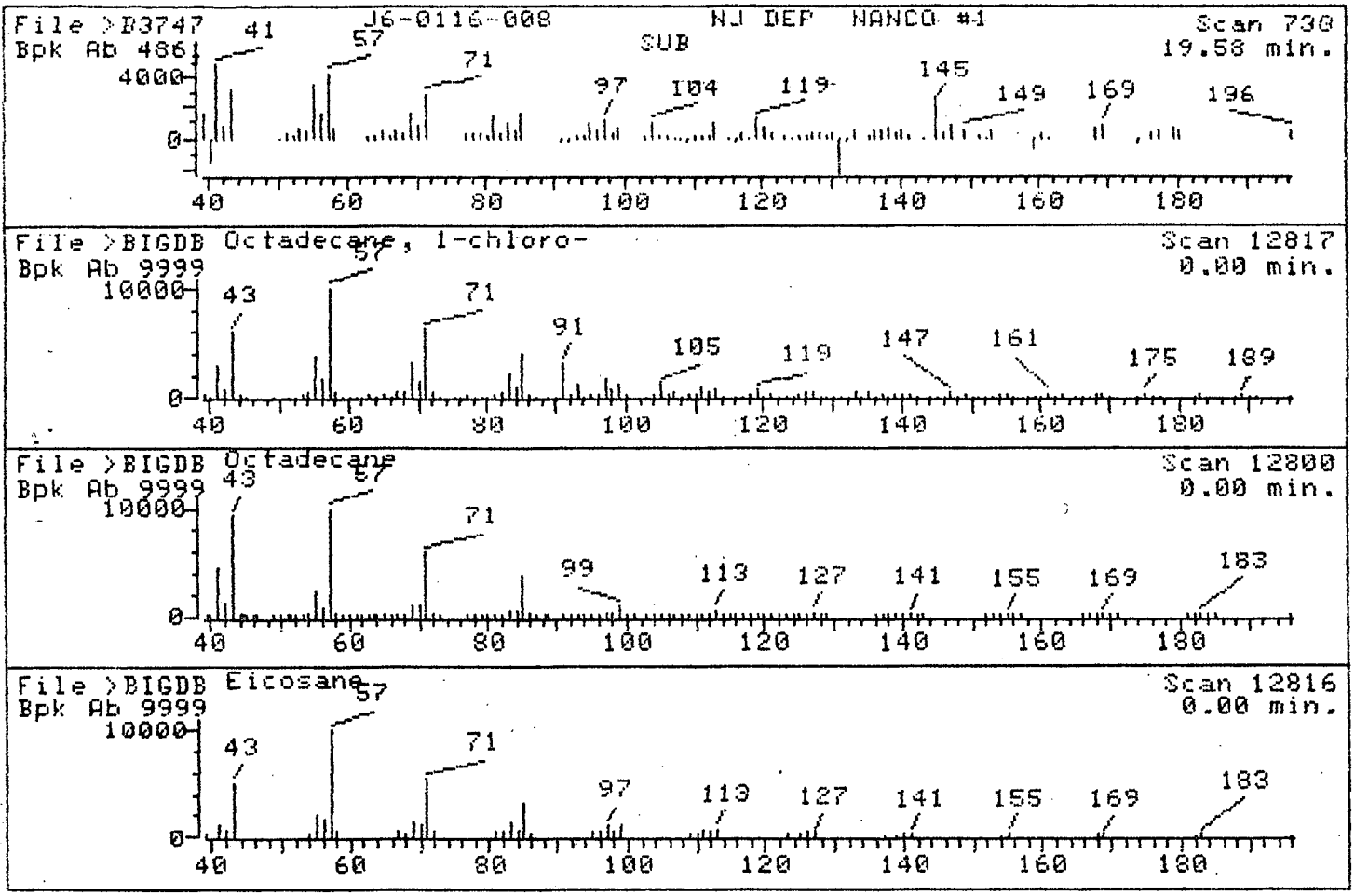


000260

1.	(Z)-2-(1'-PROPENYL)MESITYLENE	160 C12H16
2.	3-METHYLBENZALACETONE	160 C11H12O
3.	Naphthalene, 1,2,3,4-tetrahydro-2,7-dimethyl-	160 C12H16
4.	Naphthalene, 1,2,3,4-tetrahydro-2,6-dimethyl-	160 C12H16
5.	4-AMINOQUINAZOLINE	145 C8H7N3

Sample file: >B3747 Spectrum #: 730
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	51*	0	34734	"BIGDB	63	36	0	0	97	52	16	76
2.	47*	0	34710	"BIGDB	77	35	3	0	91	44	16	42
3.	34*	13065071	25517	"BIGDB	42	73	1	0	88	39	14	21
4.	25*	7524632	25516	"BIGDB	37	74	2	0	85	48	7	14
5.	25*	15018663	34650	"BIGDB	33	82	3	0	100	48	7	13

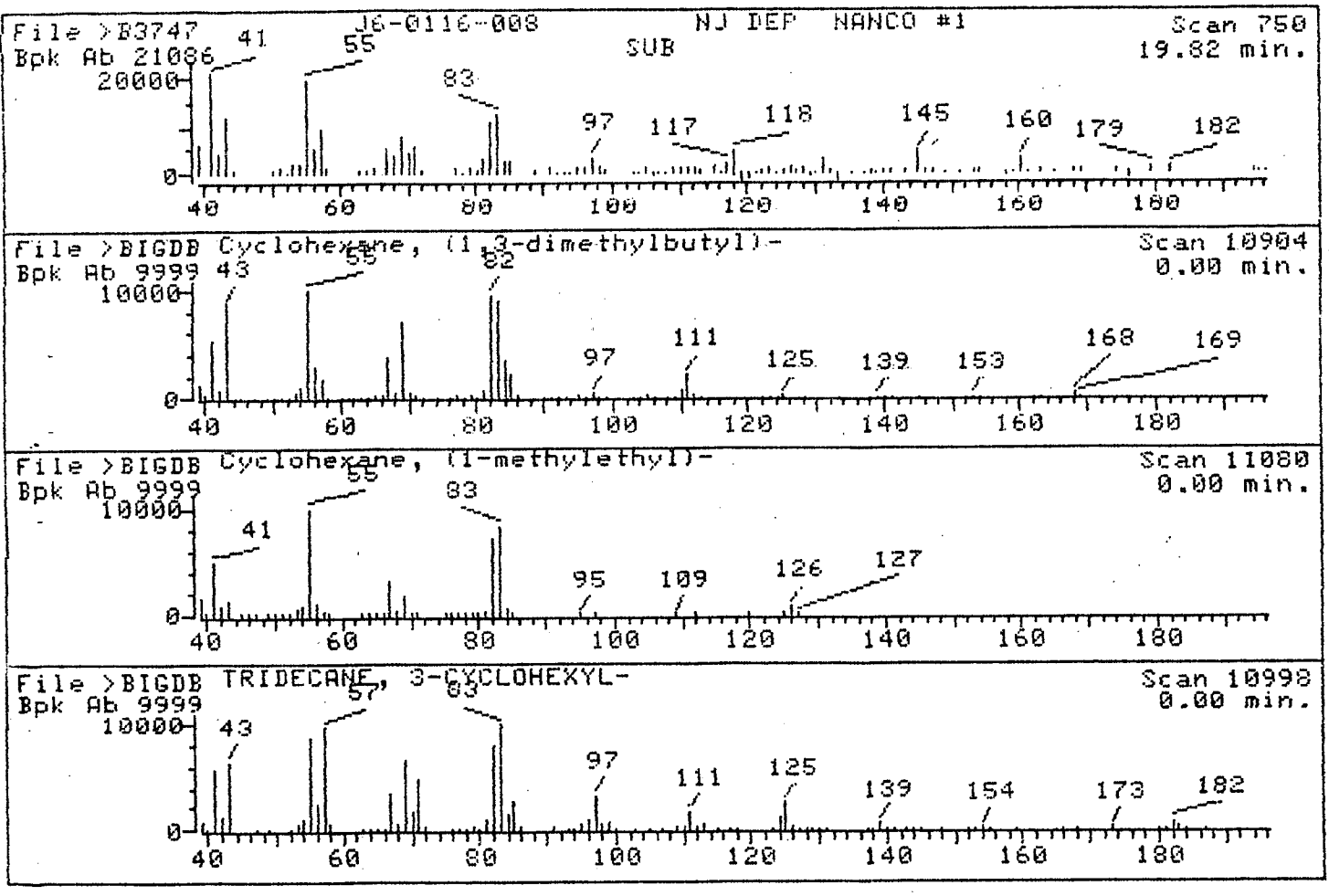


000261

1. Octadecane, 1-chloro-	288	C18H37Cl
2. Octadecane	254	C18H38
3. Eicosane	282	C20H42
4. Eicosane	282	C20H42
5. Eicosane	282	C20H42

Sample file: >B3747 Spectrum #: 738
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	15	3386332	12817	"BIGDB	64	76	2	0	72	60	3	14
2.	11	593453	12800	"BIGDB	62	63	2	0	69	65	2	13
3.	11	112958	12816	"BIGDB	69	70	2	0	87	61	2	15
4.	11	112958	12815	"BIGDB	68	71	2	0	62	64	2	15
5.	11	112958	12426	"BIGDB	61	67	2	0	83	65	2	12

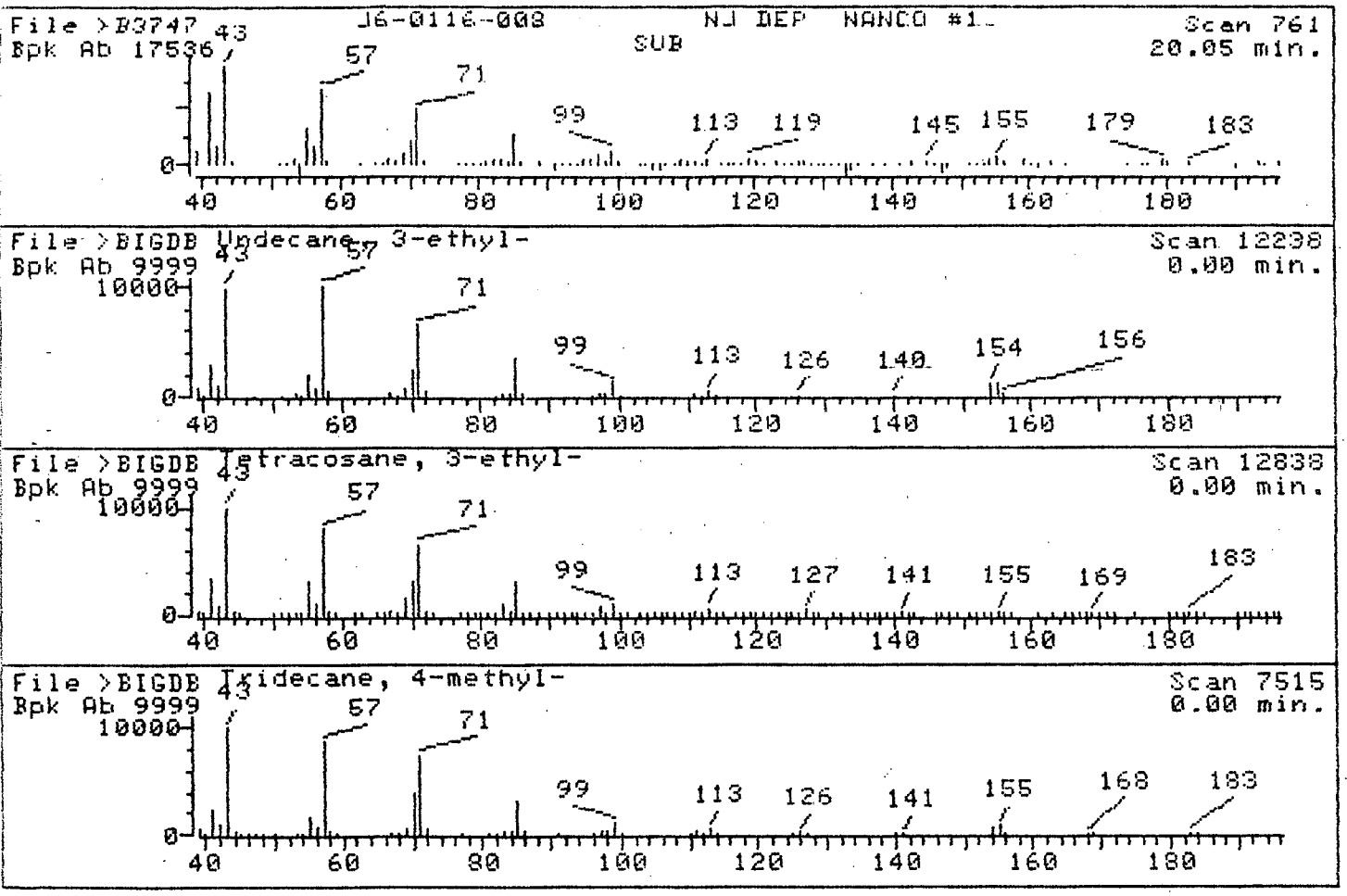


000262

1. Cyclohexane, (1,3-dimethylbutyl)-	168	C12H24
2. Cyclohexane, (1-methylethyl)-	126	C9H18
3. TRIDECANE, 3-CYCLOHEXYL-	266	C19H38
4. Cyclohexane, hexyl-	168	C12H24
5. Cyclohexane, (4-methylpentyl)-	168	C12H24

Sample file: >B3747 Spectrum #: 750
Search speed: 1 Tilting option: N No. of ion ranges searched: 53

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	35*	61142196	10904	"BIGDB	61	52	2	0	52	48	11	38
2.	32*	696297	11080	"BIGDB	43	51	0	0	70	52	9	48
3.	27	13151887	10998	"BIGDB	62	72	2	0	45	38	10	13
4.	25*	4292755	10907	"BIGDB	23	72	0	0	59	48	7	16
5.	25*	61142209	10905	"BIGDB	22	74	0	0	56	48	7	16

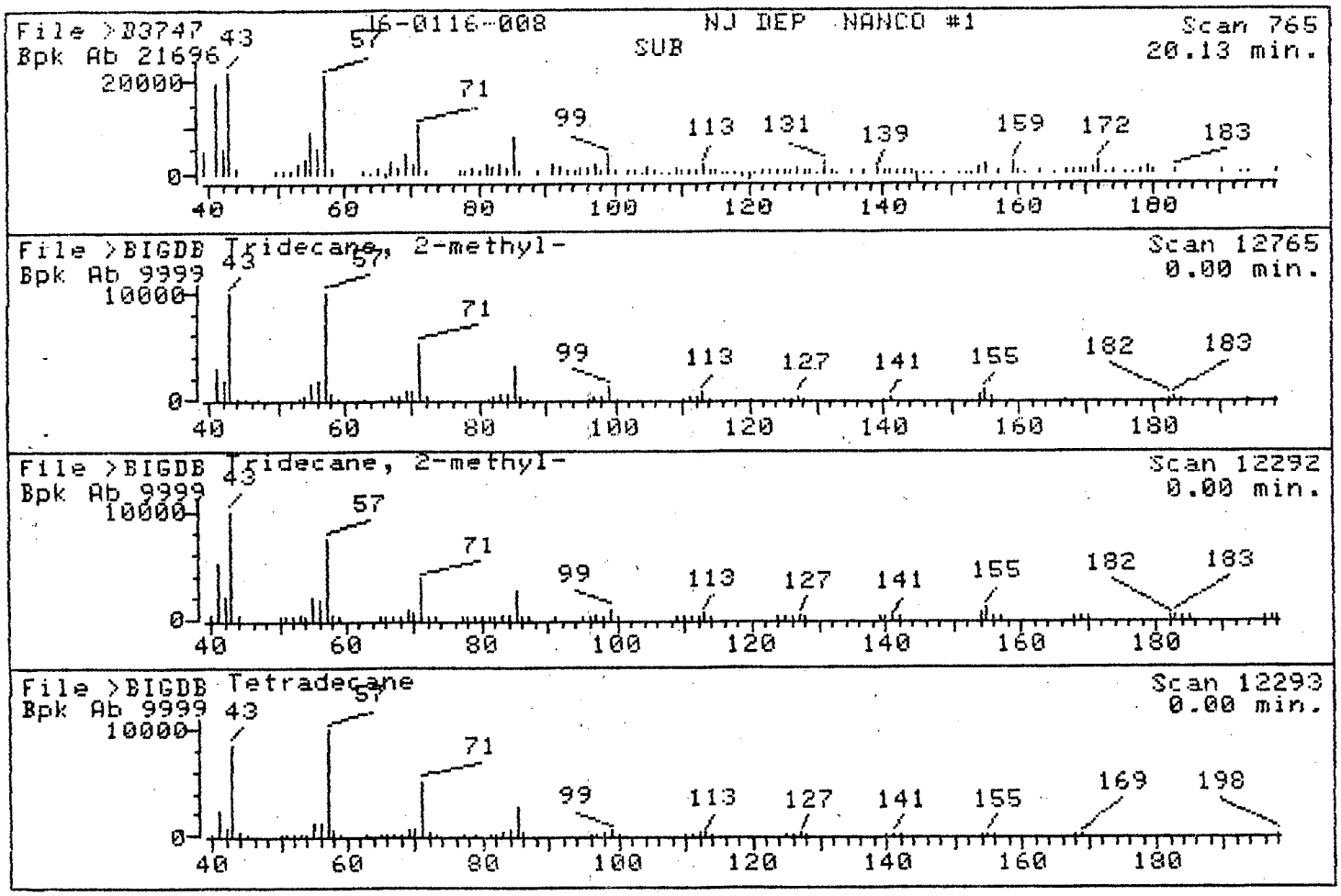


000263

1. Undecane, 3-ethyl-	184	C13H28
2. Tetracosane, 3-ethyl-	366	C26H54
3. Tridecane, 4-methyl-	198	C14H30
4. Undecane, 3,8-dimethyl-	184	C13H28
5. Nonane, 2,6-dimethyl-	156	C11H24

Sample file: >B3747 Spectrum #: 761
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	74	17312582	12238	"BIGDB	85	24	1	0	74	11	39	44
2.	70	55282172	12838	"BIGDB	74	71	2	0	66	10	42	18
3.	67	26730121	7515	"BIGDB	70	45	1	0	61	15	34	27
4.	67	17301303	12235	"BIGDB	63	45	1	0	66	14	34	21
5.	64*	17302282	7414	"BIGDB	52	39	1	0	67	25	28	40

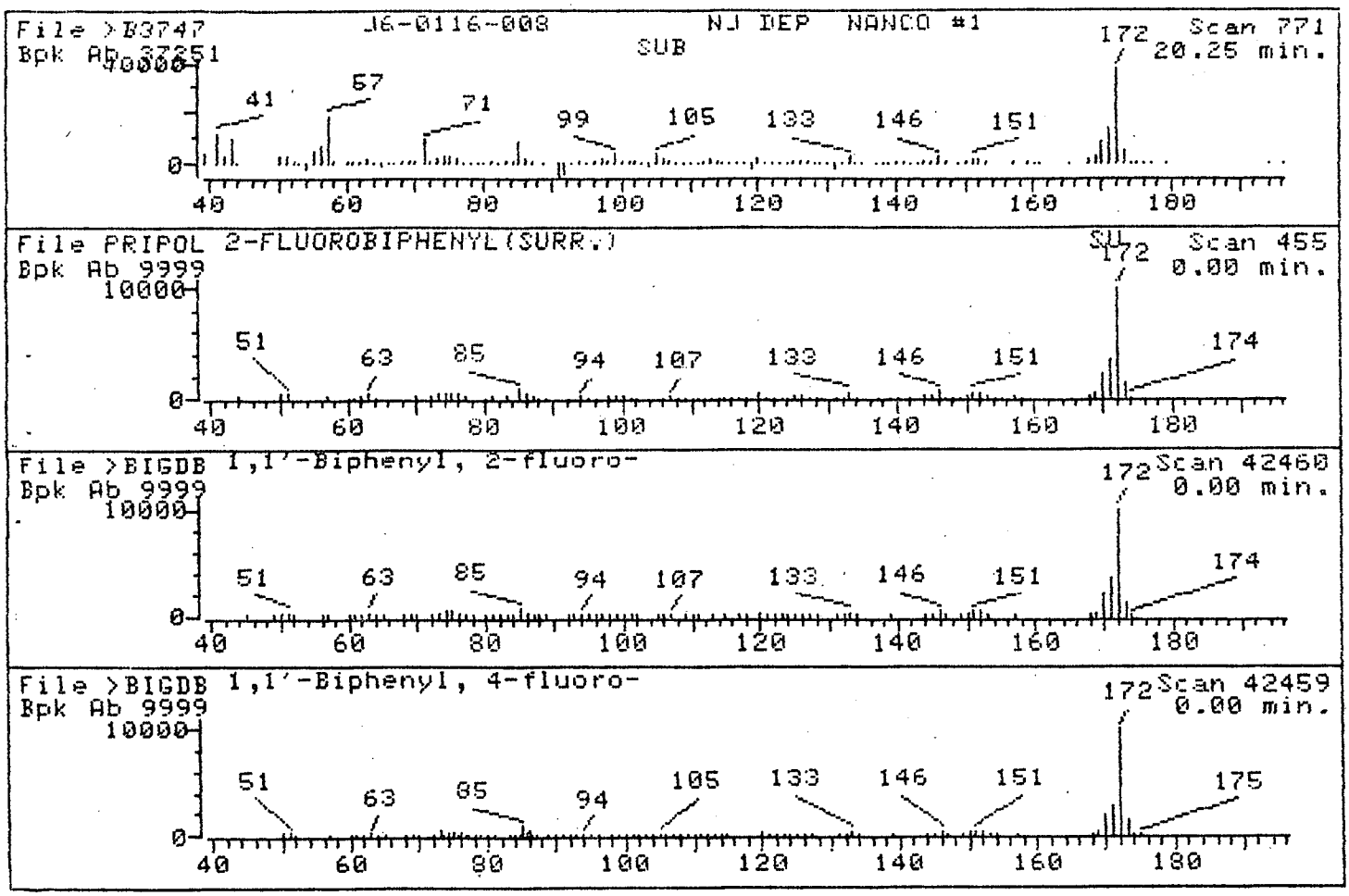


000264

1.	Tridecane, 2-methyl-	198 C14H30
2.	Tridecane, 2-methyl-	198 C14H30
3.	Tetradecane	198 C14H30
4.	Undecane, 2-methyl-	170 C12H26
5.	Tridecane, 2-methyl-	198 C14H30

Sample file: >B3747 Spectrum #: 765
Search speed: 1 Tilting option: N No. of ion ranges searched: 48

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	95*	1560969	12765	"BIGDB	88	23	0	0	91	16	60	96
2.	75*	1560969	12292	"BIGDB	84	30	2	0	97	18	35	65
3.	69*	629594	12293	"BIGDB	56	47	0	0	91	35	26	67
4.	66*	7045718	12726	"BIGDB	63	41	2	0	91	18	31	41
5.	63*	1560969	12766	"BIGDB	74	46	3	0	89	20	30	39



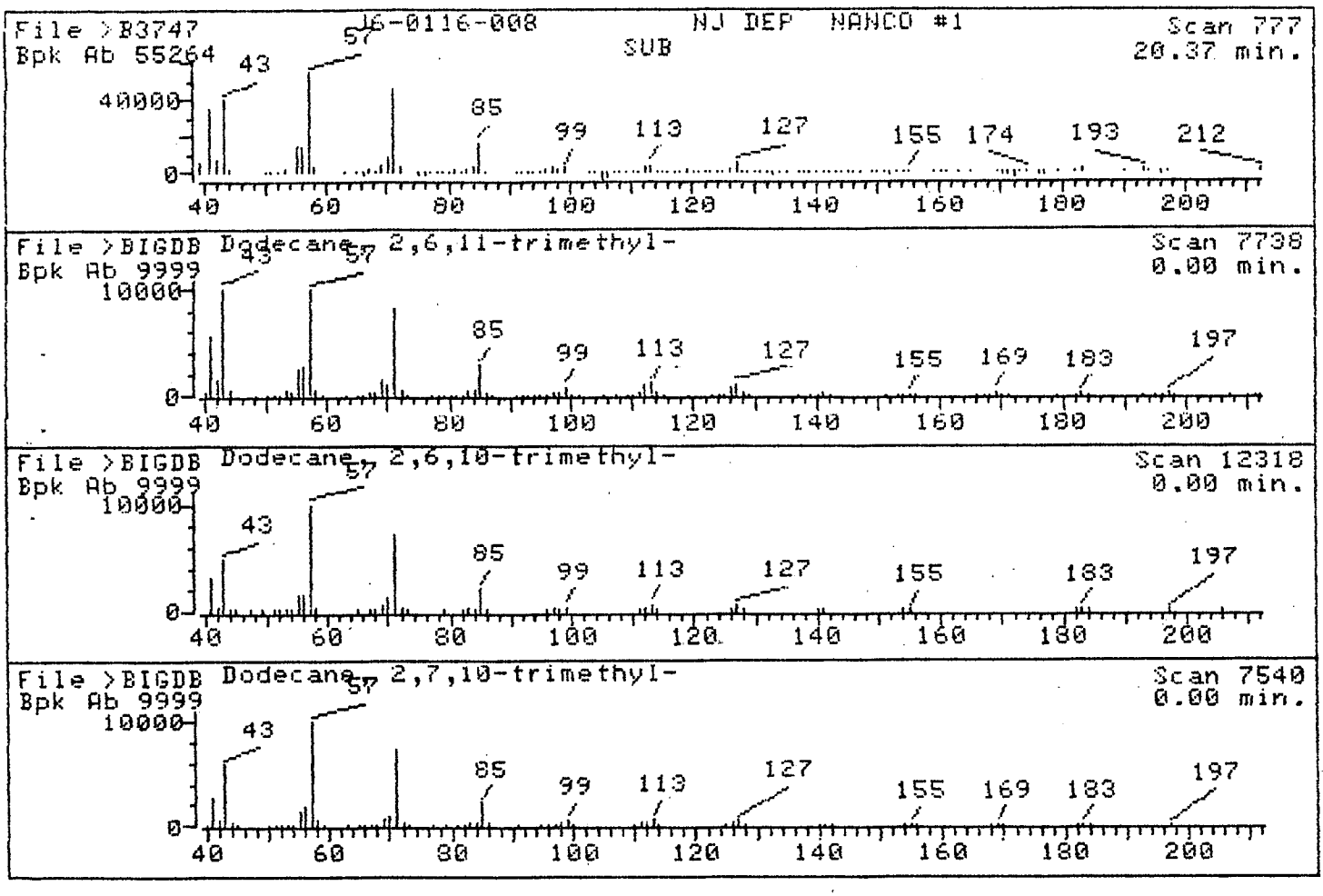
000265

16

1. 2-FLUOROBIPHENYL(SURR.) SU 172 C12H9F
   RROGATE COMPOUND BNA
   SURROGATE
2. ~~1,1'-Biphenyl, 2-fluoro-~~ 172 C12H9F
3. 1,1'-Biphenyl, 4-fluoro- 172 C12H9F
4. 2,2,6-TRIMETHYL-4,7,9-TRIOXABICYCLO[4.2.1]NONANE 172 C9H16O3
5. 2-Propenenitrile, 3-[4-(dimethylamino)phenyl]- 172 C11H12N2

Sample file: >B3747 Spectrum #: 771
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	93*	455	299	PRIPOL	84	20	0	0	97	25	53	95
2.	89*	321608	42460	"BIGDB	72	32	0	0	99	25	47	89
3.	73*	324743	42459	"BIGDB	71	33	1	0	98	26	37	71
4.	25*	0	42429	"BIGDB	24	76	3	0	357	47	7	12
5.	20*	32444636	42458	"BIGDB	31	62	3	0	100	51	5	13



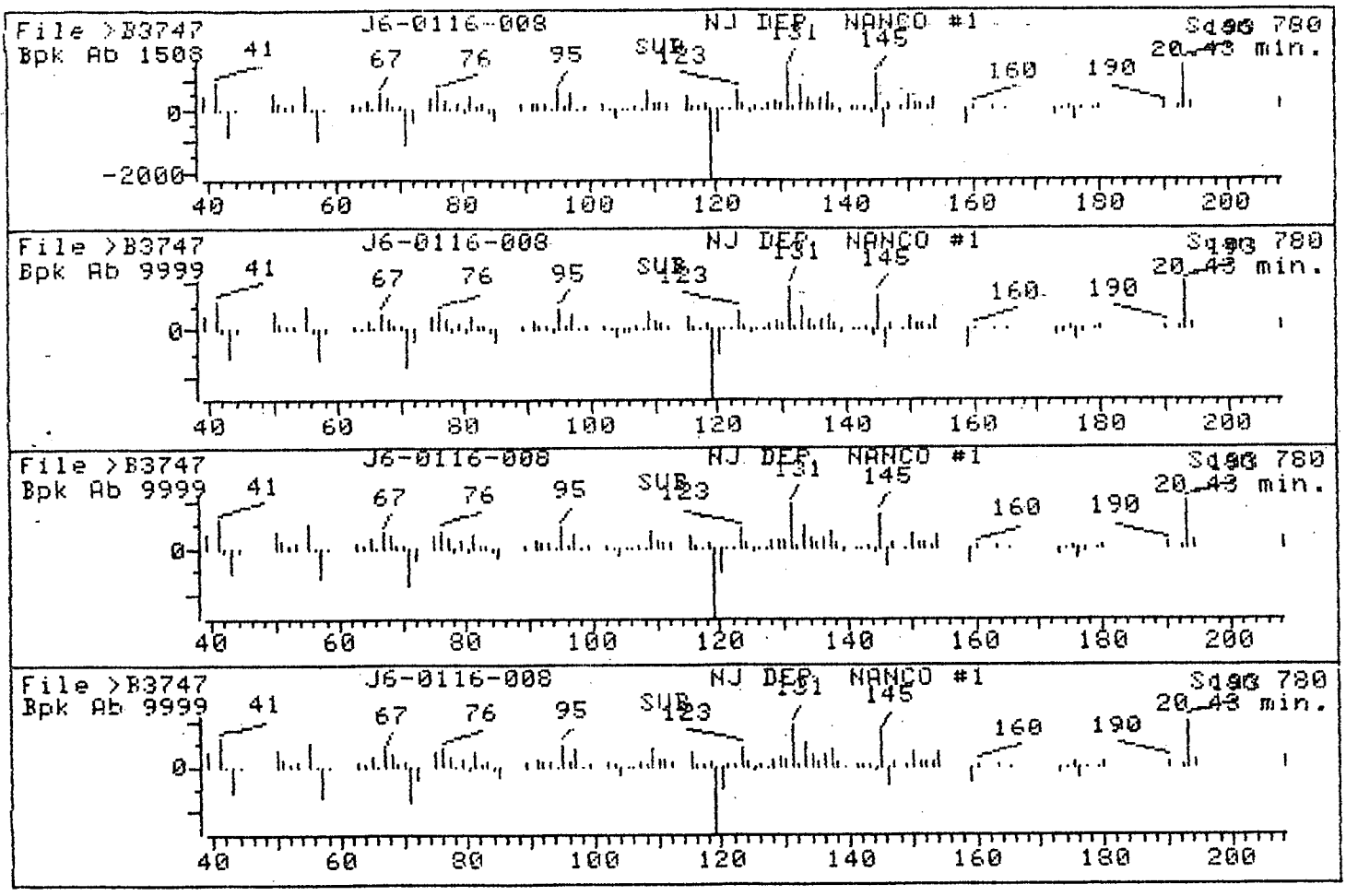
Hydrocarbon

000266

1. Dodecane, 2,6,11-trimethyl-	212	C15H32
2. Dodecane, 2,6,10-trimethyl-	212	C15H32
3. Dodecane, 2,7,10-trimethyl-	212	C15H32
4. Heptane, 3-ethyl-5-methyl-	142	C10H22
5. Nonane, 3,7-dimethyl-	156	C11H24

Sample file: >B3747 Spectrum #: 777
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

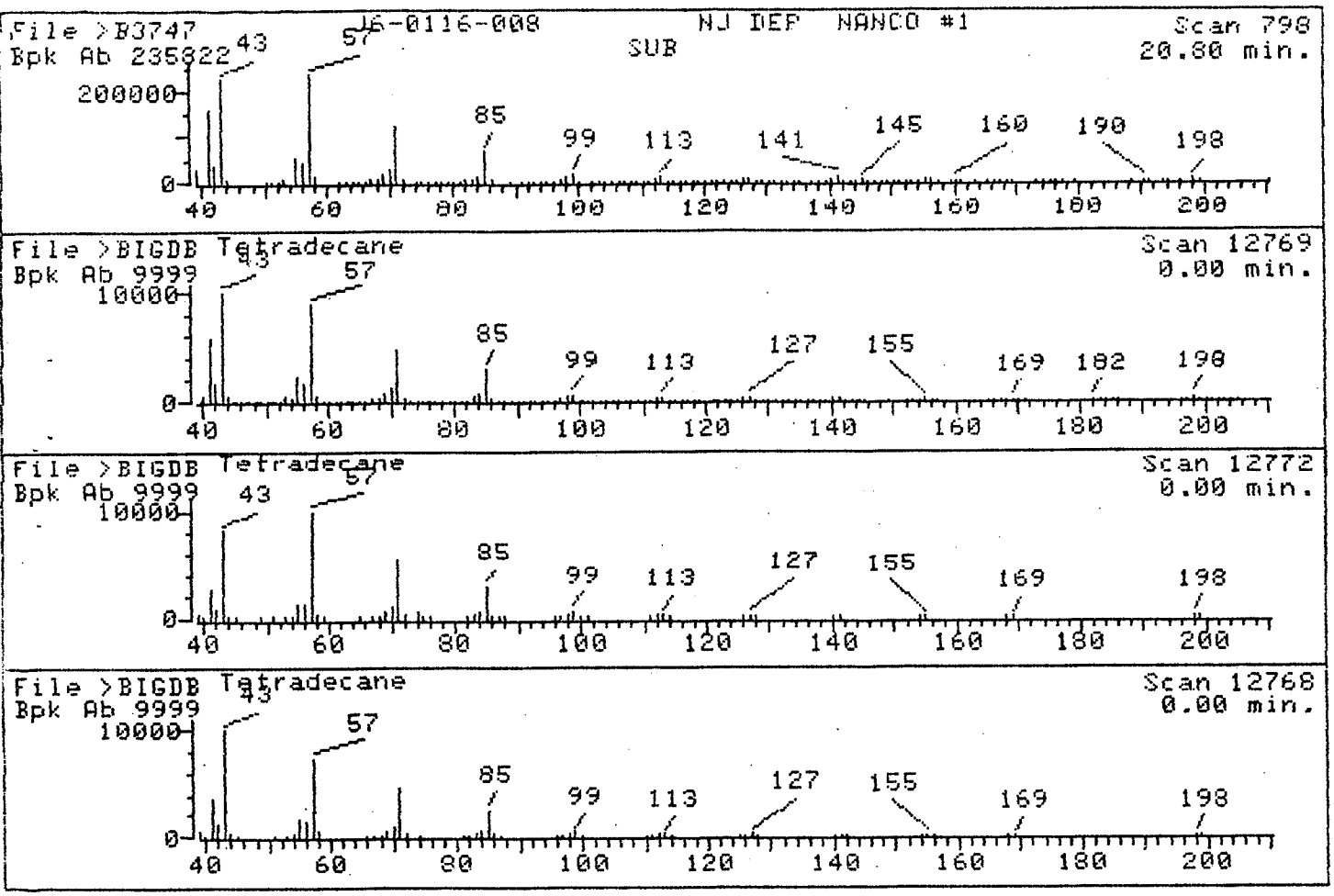
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89*	31295564	7738	"BIGDB	90	34	2	0	73	5	66	69
2.	81	3891983	12318	"BIGDB	85	21	1	0	100	8	53	49
3.	81	74645980	7540	"BIGDB	86	23	1	0	100	6	53	45
4.	80*	52896909	7369	"BIGDB	63	30	0	0	72	23	41	76
5.	79	17302328	12095	"BIGDB	73	13	1	0	86	7	48	36



000267

Sample file: >B3747 Spectrum #: 780

No data base entries were retrieved.

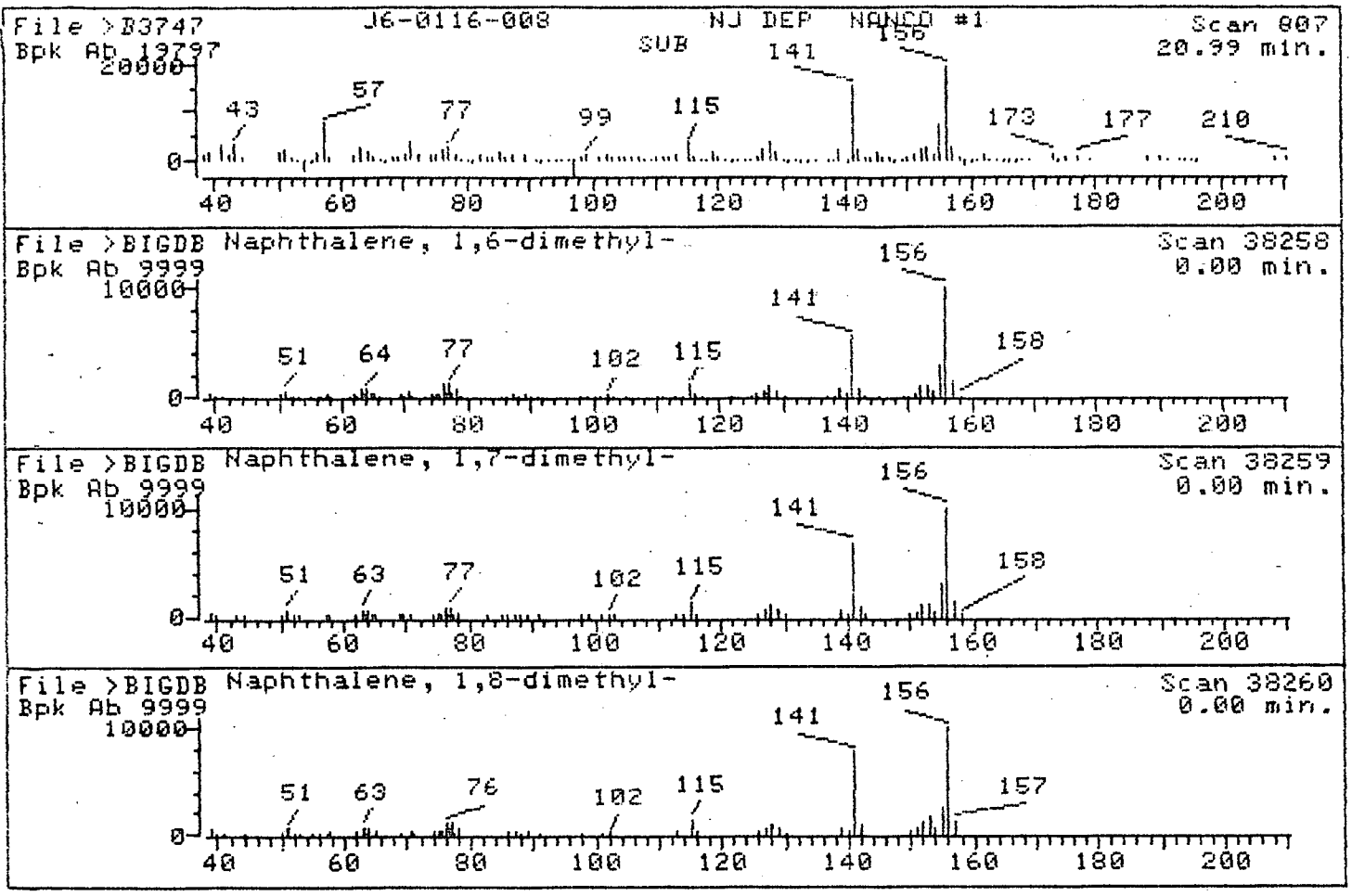


000268

1. Tetradecane 198 C14H30
2. Tetradecane 198 C14H30
3. Tetradecane 198 C14H30
4. Tetradecane 198 C14H30
5. Tridecane 184 C13H28

Sample file: >B3747 Spectrum #: 798
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	97*	629594	12769	"BIGDB	100	9	0	0	93	2	72	97
2.	95*	629594	12772	"BIGDB	98	10	1	0	99	2	72	95
3.	95*	629594	12768	"BIGDB	87	21	0	0	95	2	72	95
4.	93*	629594	12293	"BIGDB	72	31	0	0	97	2	68	89
5.	89	629505	12750	"BIGDB	93	14	1	0	87	4	66	63

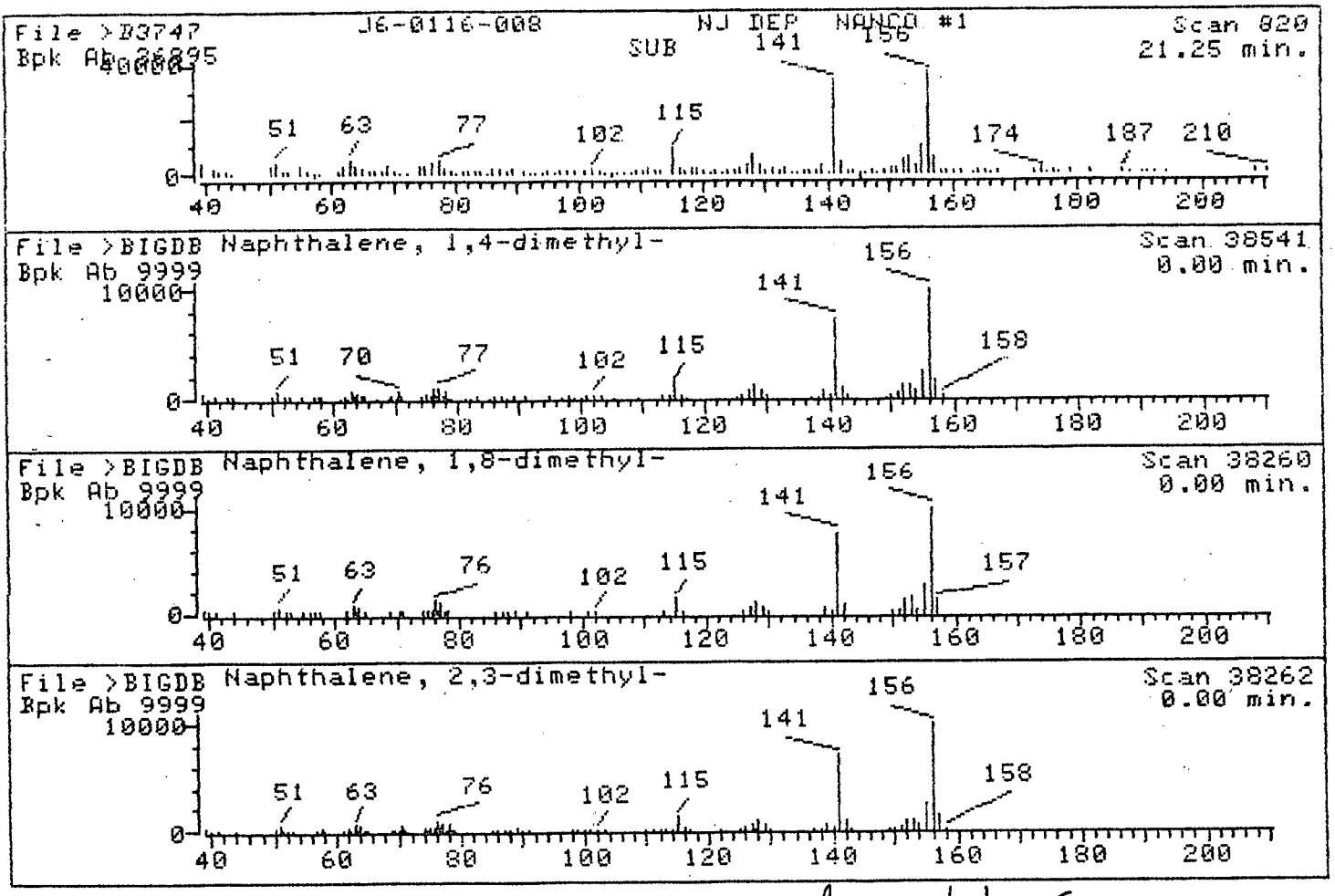


000269

1.	Naphthalene, 1,6-dimethyl-	156 C12H12
2.	Naphthalene, 1,7-dimethyl-	156 C12H12
3.	Naphthalene, 1,8-dimethyl-	156 C12H12
4.	Naphthalene, 2,3-dimethyl-	156 C12H12
5.	Naphthalene, 1,5-dimethyl-	156 C12H12

Sample file: >B3747 Spectrum #: 807
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	97*	575439	38258	"BIGDB	101	7	0	0	100	0	72	97
2.	97*	575371	38259	"BIGDB	100	8	0	0	100	0	72	97
3.	97*	569415	38260	"BIGDB	100	10	0	0	87	0	72	97
4.	97*	581408	38262	"BIGDB	97	9	0	0	93	0	72	97
5.	96*	571619	38257	"BIGDB	101	8	1	0	95	4	72	96



isomer of dimethyl naphthalene

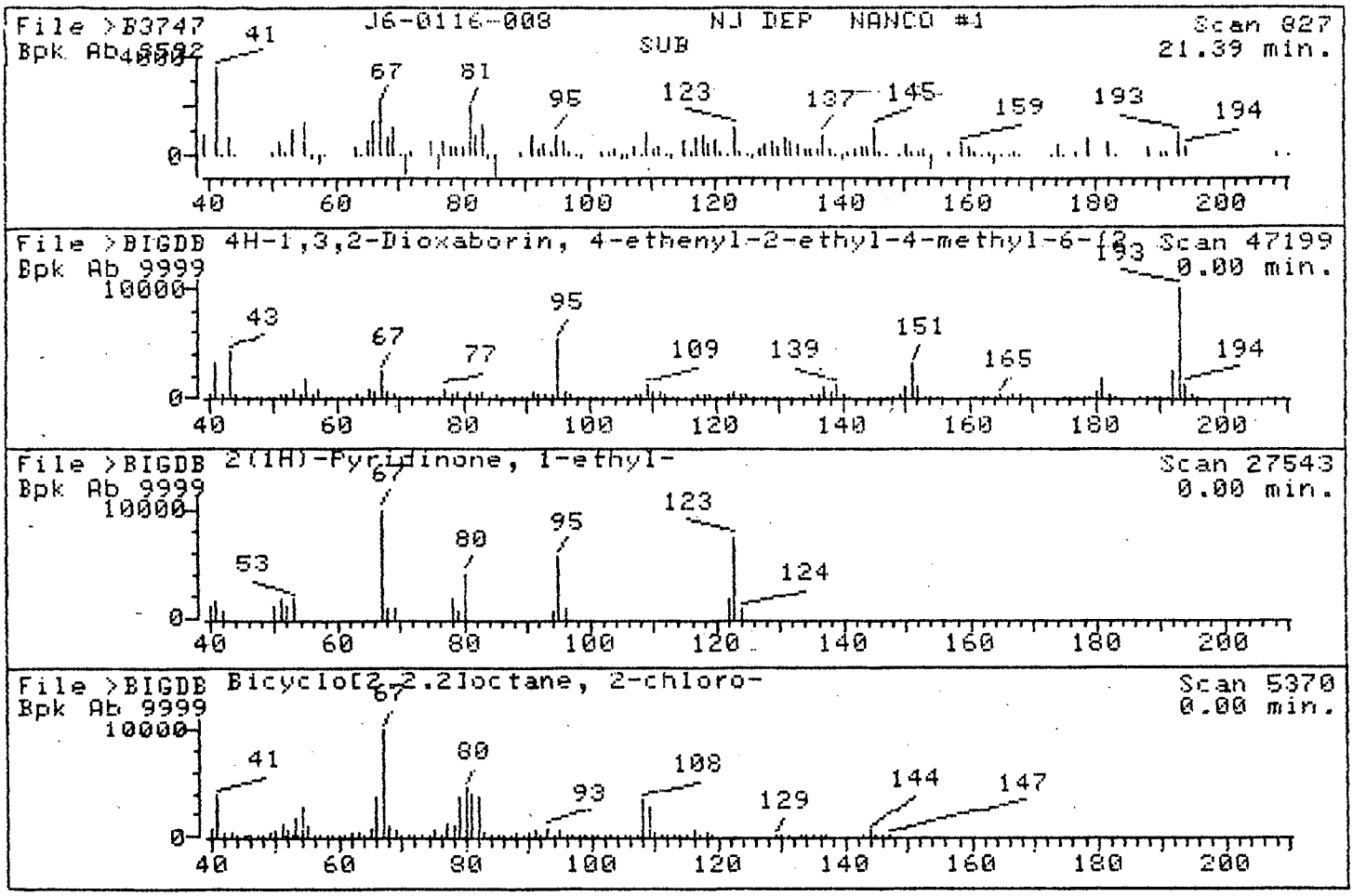
000270

1. Naphthalene, 1,4-dimethyl-	156	C12H12
2. Naphthalene, 1,8-dimethyl-	156	C12H12
3. Naphthalene, 2,3-dimethyl-	156	C12H12
4. Naphthalene, 1,7-dimethyl-	156	C12H12
5. Naphthalene, 1,3-dimethyl-	156	C12H12

16

Sample file: >B3747 Spectrum #: 820
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	97*	571584	38541	"BIGDB	97	15	0	0	100	3	72	97
2.	97*	569415	38260	"BIGDB	95	15	0	0	94	3	72	97
3.	96*	581408	38262	"BIGDB	92	14	0	0	100	3	72	96
4.	96*	575371	38259	"BIGDB	93	15	0	0	100	3	72	96
5.	95*	575417	38256	"BIGDB	94	13	1	0	94	3	72	93

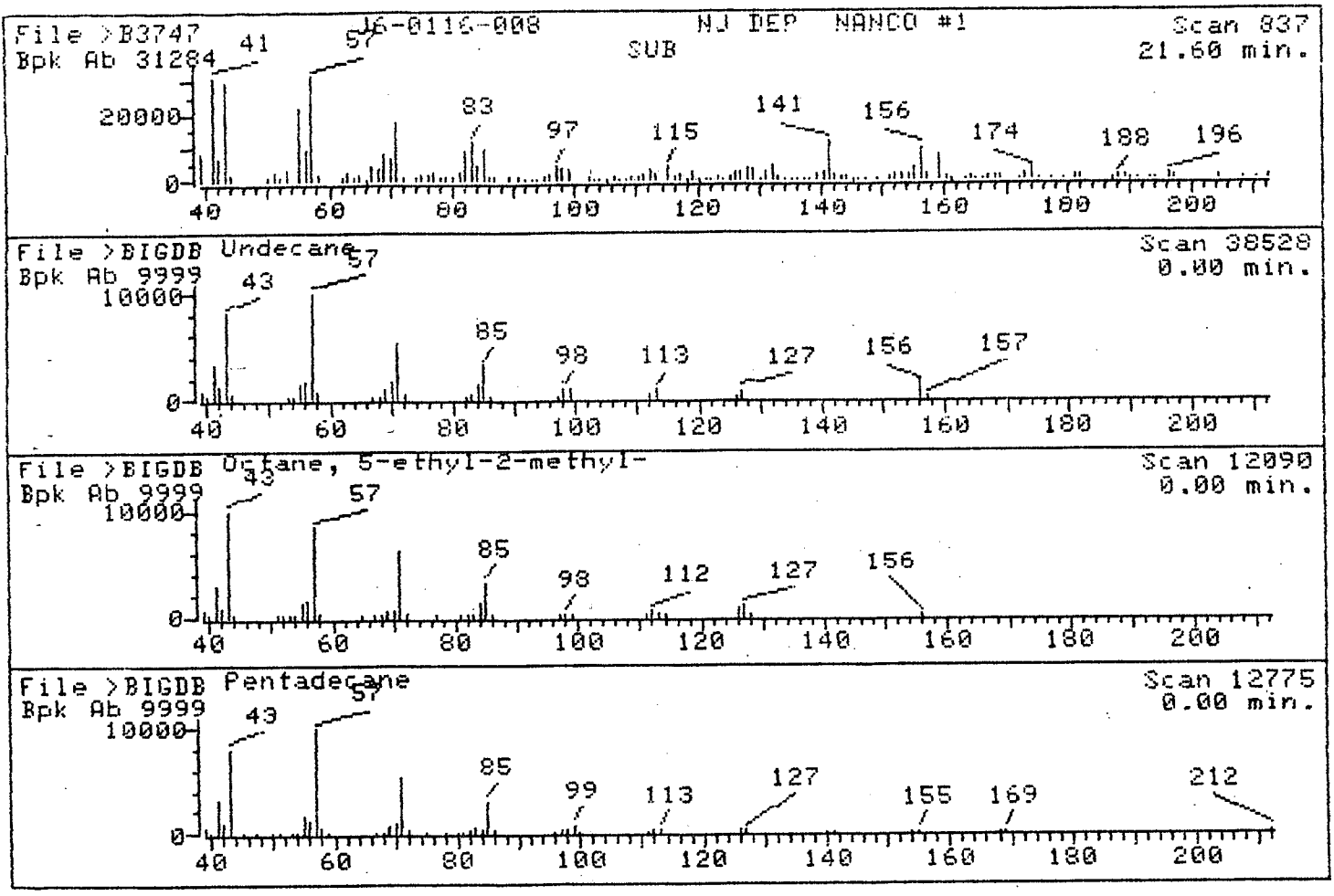


000271

1.	4H-1,3,2-Dioxaborin, 4-ethenyl-2-ethyl-4-methyl-6-(2-methylpropyl)-	208	C12H21BO2
2.	2(1H)-Pyridinone, 1-ethyl-	123	C7H9NO
3.	Bicyclo[2.2.2]octane, 2-chloro-	144	C8H13Cl
4.	Acetic acid, trifluoro-, bicyclo[2.2.1]hept-2-yl est	208	C9H11F3O2
5.	1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	208	C15H28

Sample file: >B3747 Spectrum #: 827
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	29*	74630049	47199	"BIGDB	24	109	3	0	234	34	12	12
2.	15*	13337796	27543	"BIGDB	40	57	2	0	39	60	3	17
3.	15*	33649795	5370	"BIGDB	22	94	3	0	55	59	3	12
4.	15*	54934984	5536	"BIGDB	31	112	3	0	68	60	3	13
5.	11*	54832836	47211	"BIGDB	27	79	3	0	23	64	2	13



Hydrocarb

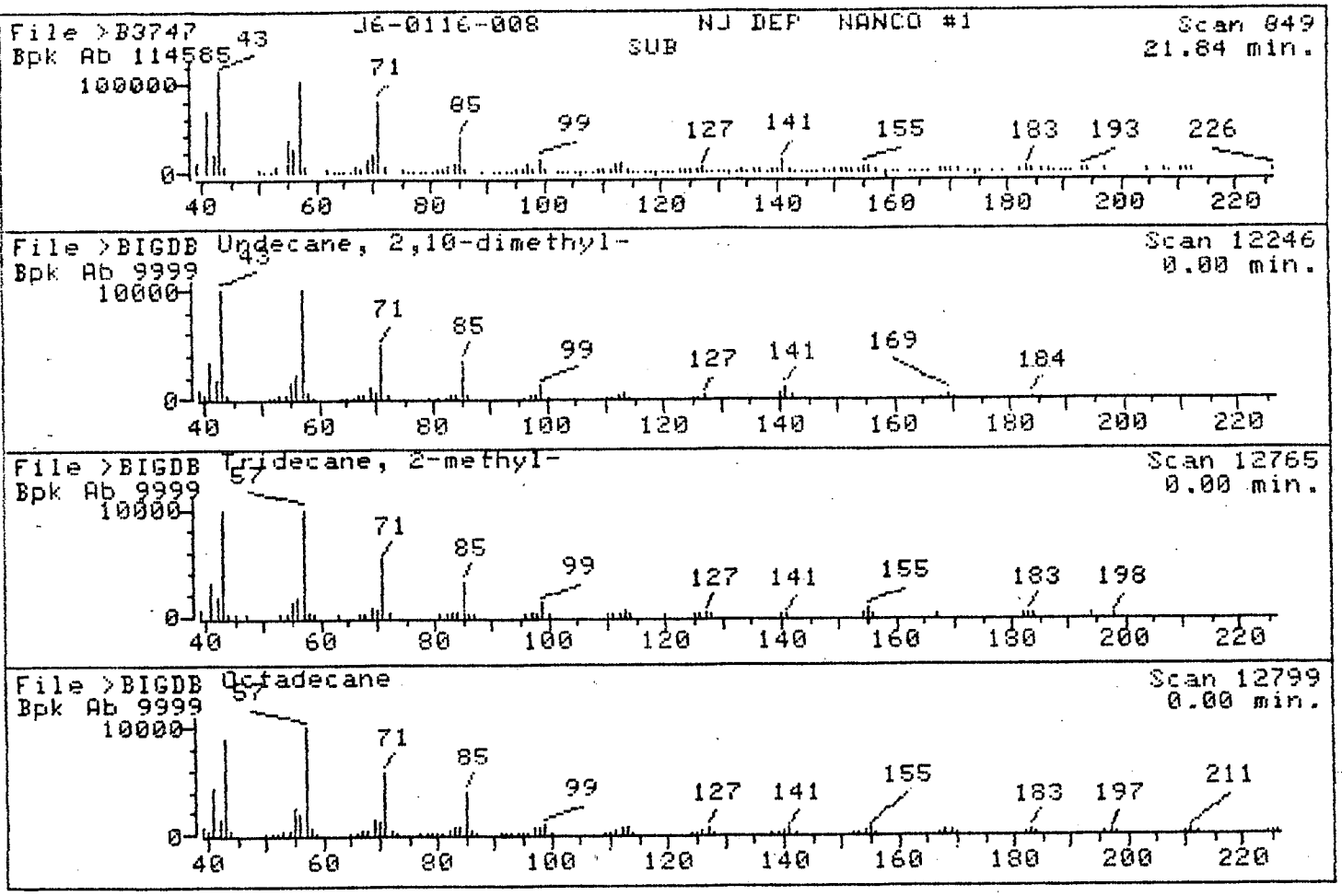
/16

000072

1. Undecane	156	C11H24
2. Octane, 5-ethyl-2-methyl-	156	C11H24
3. Pentadecane	212	C15H32
4. Nonane, 3,7-dimethyl-	156	C11H24
5. Decane, 3-methyl-	156	C11H24

Sample file: >B3747 Spectrum #: 837
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	49*	1120214	38528	"BIGDB	77	31	1	0	83	51	16	74
2.	33*	62016186	12090	"BIGDB	60	38	0	0	76	60	12	73
3.	31*	629629	12775	"BIGDB	52	54	0	0	98	60	8	63
4.	31*	17302328	12095	"BIGDB	52	34	0	0	80	60	8	63
5.	31*	13151343	12091	"BIGDB	54	40	0	0	73	60	8	66

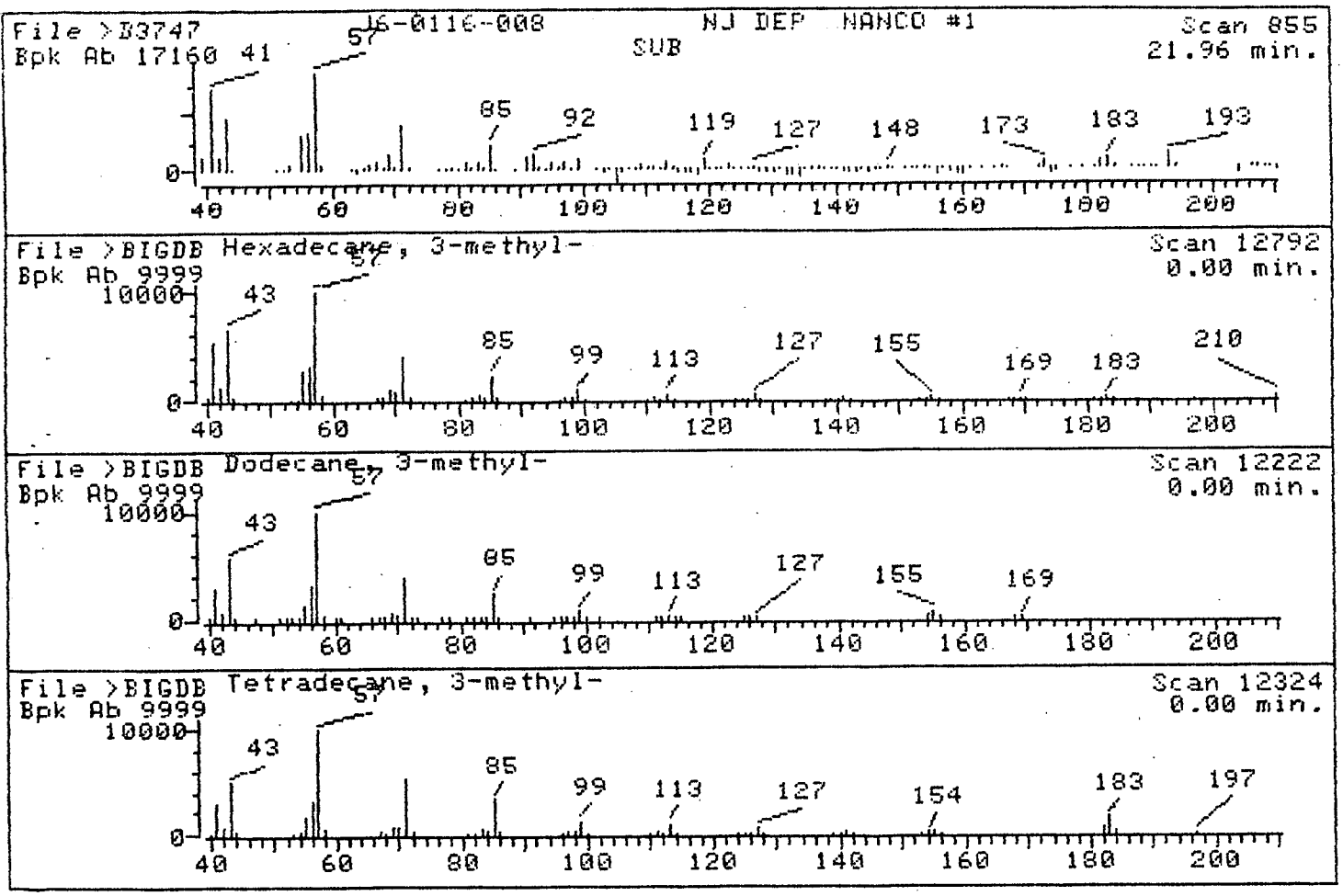


000273

1. Undecane, 2,10-dimethyl- 184 C13H28
2. Tridecane, 2-methyl- 198 C14H30
3. Octadecane 254 C18H38
4. Undecane, 3,8-dimethyl- 184 C13H28
5. Dodecane, 2-methyl-8-propyl- 226 C16H34

Sample file: >B3747 Spectrum #: 849
Search speed: 1 Tilting option: N No. of ion ranges searched: 45

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	93*	17301278	12246	"BIGDB	75	34	0	0	72	18	60	93
2.	86	1560969	12765	"BIGDB	84	27	2	0	89	4	60	31
3.	83	593453	12799	"BIGDB	88	45	2	0	79	3	57	25
4.	83	17301303	12235	"BIGDB	74	34	2	0	82	3	57	24
5.	83*	55045073	12343	"BIGDB	76	52	2	0	75	8	54	59

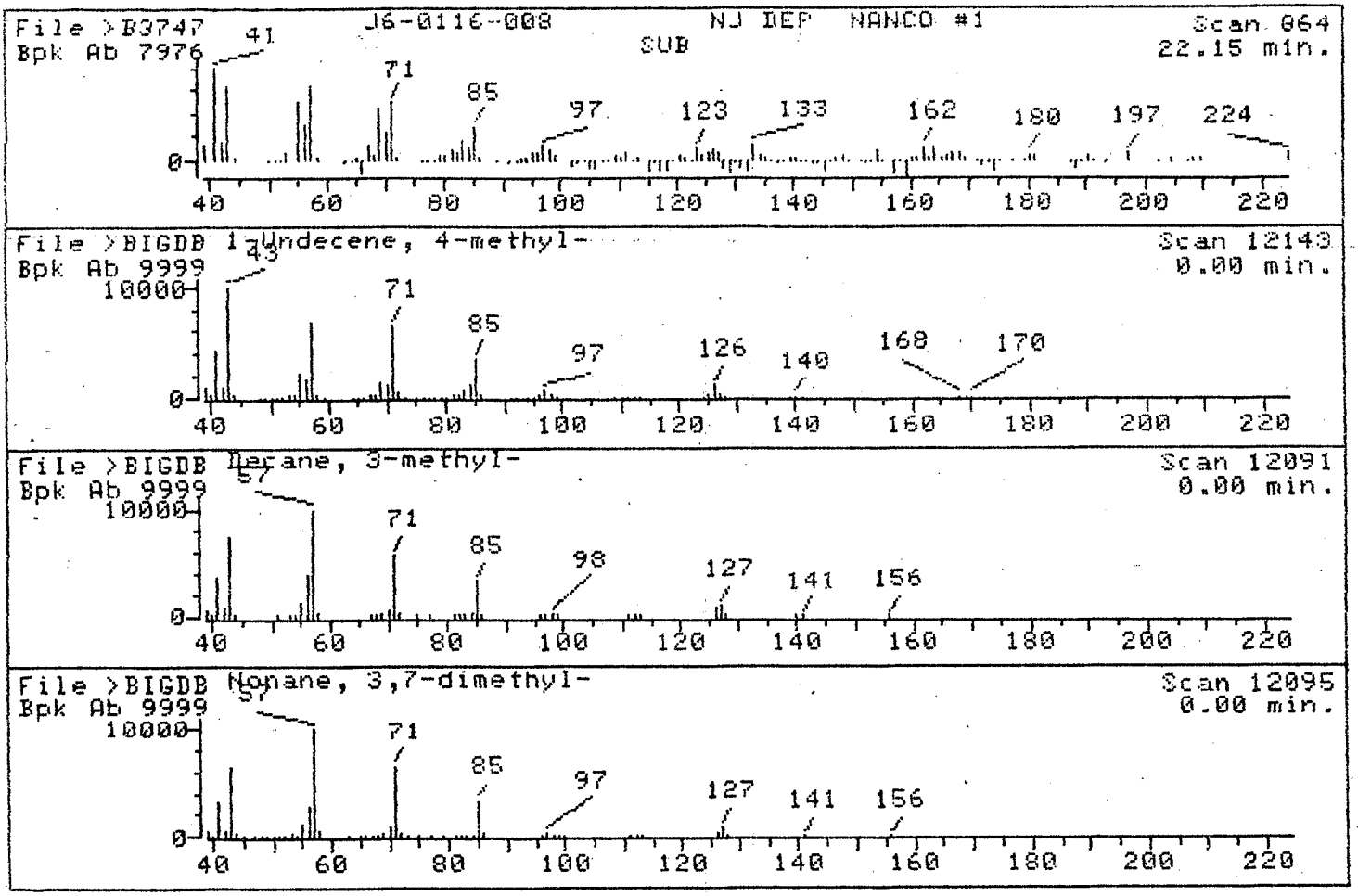


000274

1. Hexadecane, 3-methyl-	240	C17H36
2. Dodecane, 3-methyl-	184	C13H28
3. Tetradecane, 3-methyl-	212	C15H32
4. Undecane, 2,9-dimethyl-	184	C13H28
5. Octacosane	394	C28H58

Sample file: >B3747 Spectrum #: 855
Search speed: 1 Tilting option: N No. of ion ranges searched: 49

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	43	6418435	12792	"BIGDB	76	37	2	0	100	29	19	21
2.	38	17312571	12222	"BIGDB	62	37	2	0	92	33	16	21
3.	35	18435228	12324	"BIGDB	73	40	2	0	72	35	12	18
4.	33	17301267	12236	"BIGDB	59	42	2	0	100	33	12	16
5.	30	630024	12848	"BIGDB	73	71	2	0	71	45	8	18

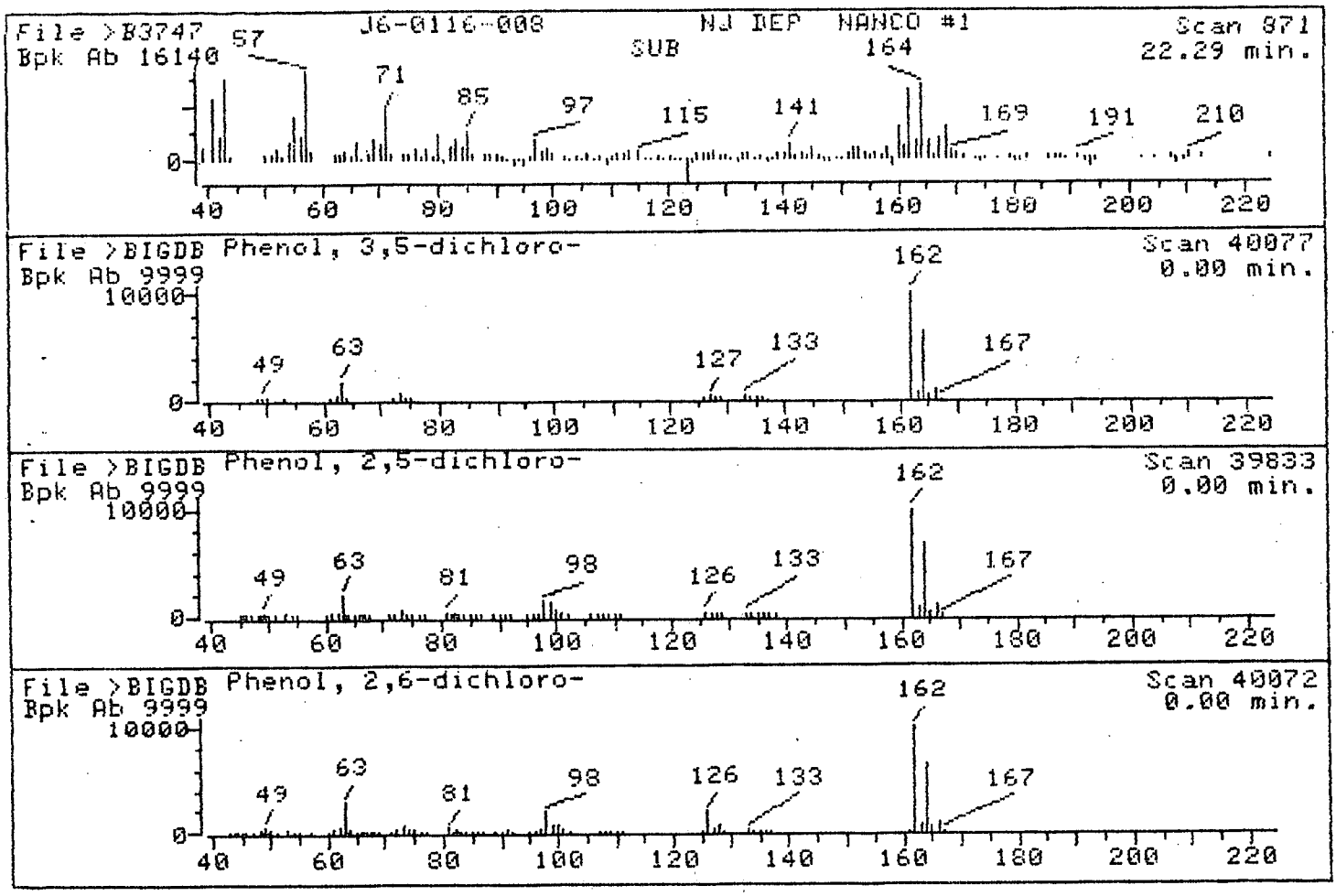


000275

1.	1-Undecene, 4-methyl-	168 C12H24
2.	Decane, 3-methyl-	156 C11H24
3.	Nonane, 3,7-dimethyl-	156 C11H24
4.	Undecane, 4-methyl-	170 C12H26
5.	Nonane, 5-(2-methylpropyl)-	184 C13H28

Sample file: >B3747 Spectrum #: 864
Search speed: 1 Tilting option: N No. of ion ranges searched: 53

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	56*	74630390	12143	"BIGDB	49	50	0	0	77	44	17	59
2.	36	13151343	12091	"BIGDB	61	33	1	0	77	44	12	27
3.	25	17302328	12095	"BIGDB	39	47	2	0	79	50	7	13
4.	25	2980690	12165	"BIGDB	48	56	1	0	74	46	7	12
5.	25	62185539	12248	"BIGDB	38	54	1	0	49	44	8	13

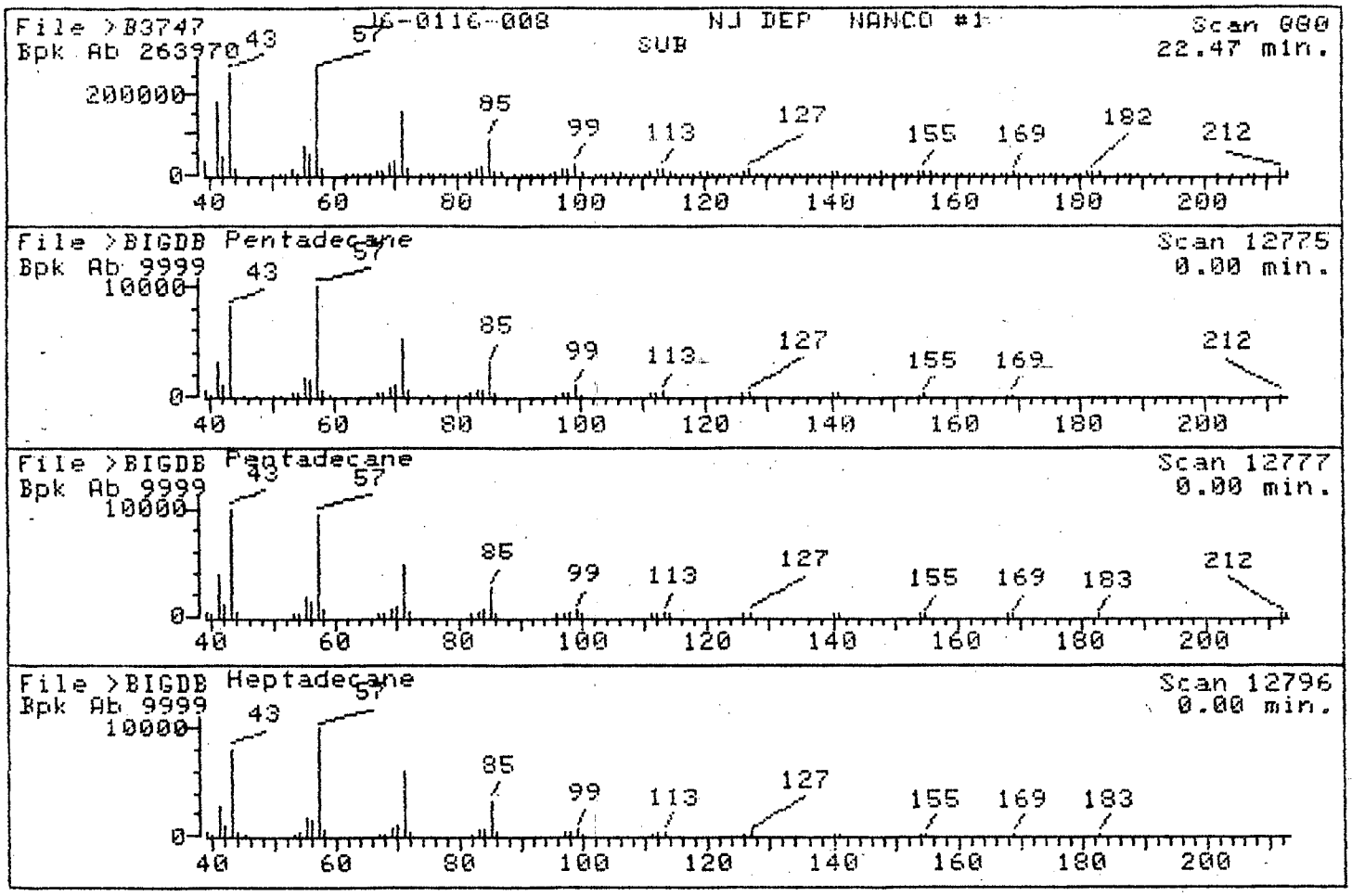


000276

1.	Phenol, 3,5-dichloro-	162 C6H4Cl2O
2.	Phenol, 2,5-dichloro-	162 C6H4Cl2O
3.	Phenol, 2,6-dichloro-	162 C6H4Cl2O
4.	Phenol, 2,4-dichloro-	162 C6H4Cl2O
5.	Phenol, 2,4-dichloro-	162 C6H4Cl2O

Sample file: >B3747 Spectrum #: 871
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	11*	591355	40077	"BIGDB	31	66	2	0	79	63	2	14
2.	11*	583788	39833	"BIGDB	34	72	2	0	79	63	2	14
3.	11*	87650	40072	"BIGDB	32	76	2	0	79	63	2	14
4.	11*	120832	40069	"BIGDB	27	79	2	0	79	63	2	14
5.	11*	179	267	PRIPOL	27	79	2	0	79	63	2	14

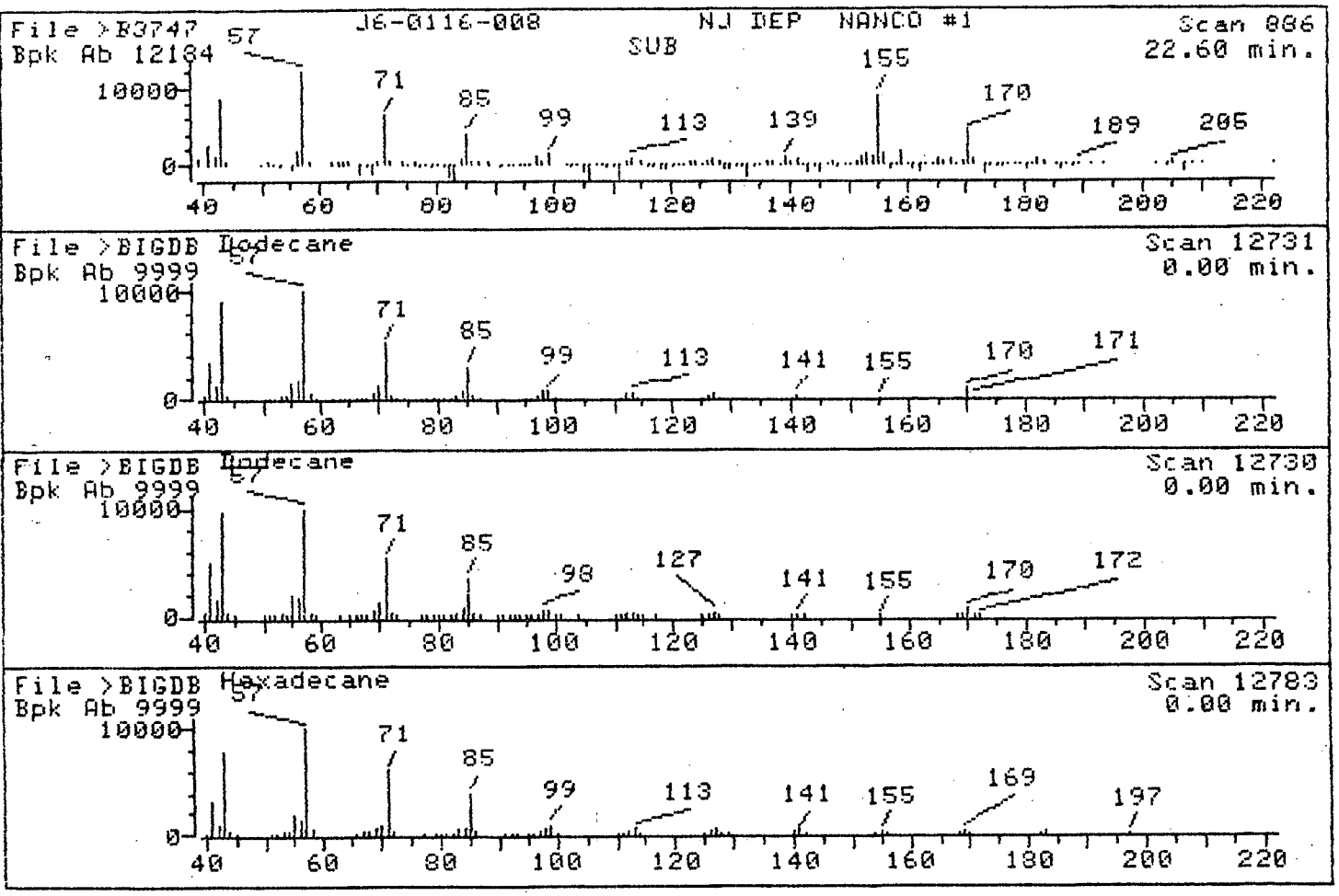


000277

1. Pentadecane	212	C15H32
2. Pentadecane	212	C15H32
3. Heptadecane	240	C17H36
4. Hexadecane	226	C16H34
5. Pentadecane	212	C15H32

Sample file: >B3747 Spectrum #: 880
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	94*	629629	12775	"BIGDB	92	14	1	0	100	0	72	92
2.	93*	629629	12777	"BIGDB	86	23	1	0	96	5	68	83
3.	89	629787	12796	"BIGDB	100	11	1	0	93	1	66	72
4.	89	544763	12354	"BIGDB	92	15	1	0	92	1	66	61
5.	89*	629629	12776	"BIGDB	79	30	1	0	74	2	66	76

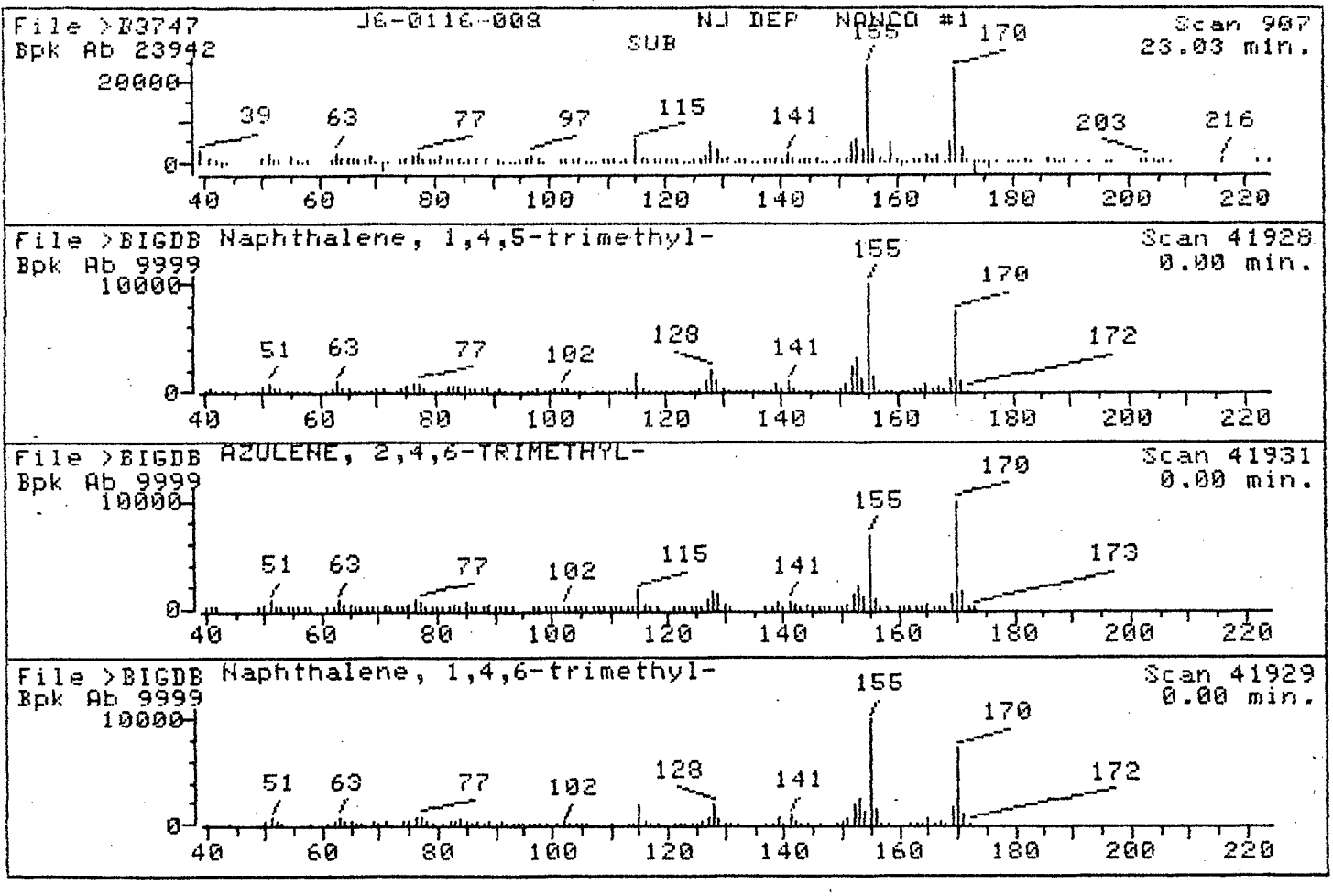


000278

1.	Dodecane	170 C12H26
2.	Dodecane	170 C12H26
3.	Hexadecane	226 C16H34
4.	Pentadecane	212 C15H32
5.	Hexacosane	366 C26H54

Sample file: >B3747 Spectrum #: 886
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	53*	112403	12731	"BIGDB	64	35	1	0	69	46	14	63
2.	35*	112403	12730	"BIGDB	55	46	2	0	72	46	11	32
3.	30	544763	12783	"BIGDB	81	39	2	0	83	46	10	22
4.	30	629629	12775	"BIGDB	70	36	2	0	87	46	10	23
5.	30	630013	12505	"BIGDB	79	55	2	0	91	46	10	21

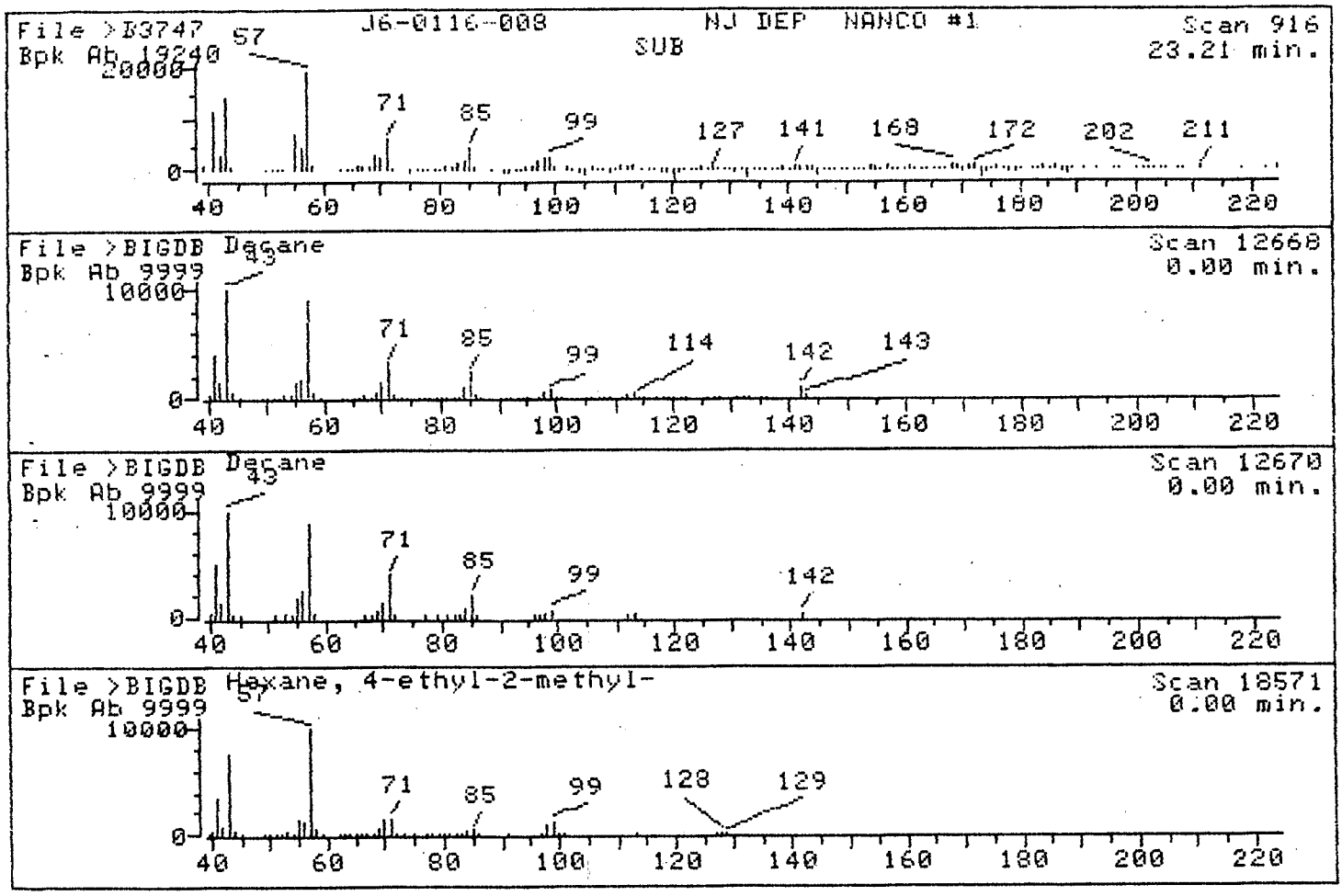


000279

1. Naphthalene, 1,4,5-trimethyl-	170	C13H14
2. AZULENE, 2,4,6-TRIMETHYL-	170	C13H14
3. Naphthalene, 1,4,6-trimethyl-	170	C13H14
4. Naphthalene, 1,6,7-trimethyl-	170	C13H14
5. METHYL-ETHYL-NAPHTALENE	170	C13H14

Sample file: >B3747 Spectrum #: 907
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	94*	2131411	41928	"BIGDB	94	24	0	0	67	25	53	96
2.	93*	0	41931	"BIGDB	88	26	0	0	91	27	57	96
3.	93*	2131422	41929	"BIGDB	82	37	0	0	69	24	53	94
4.	81*	2245387	41926	"BIGDB	68	40	0	0	96	31	40	83
5.	76*	0	41932	"BIGDB	75	41	2	0	97	13	40	57

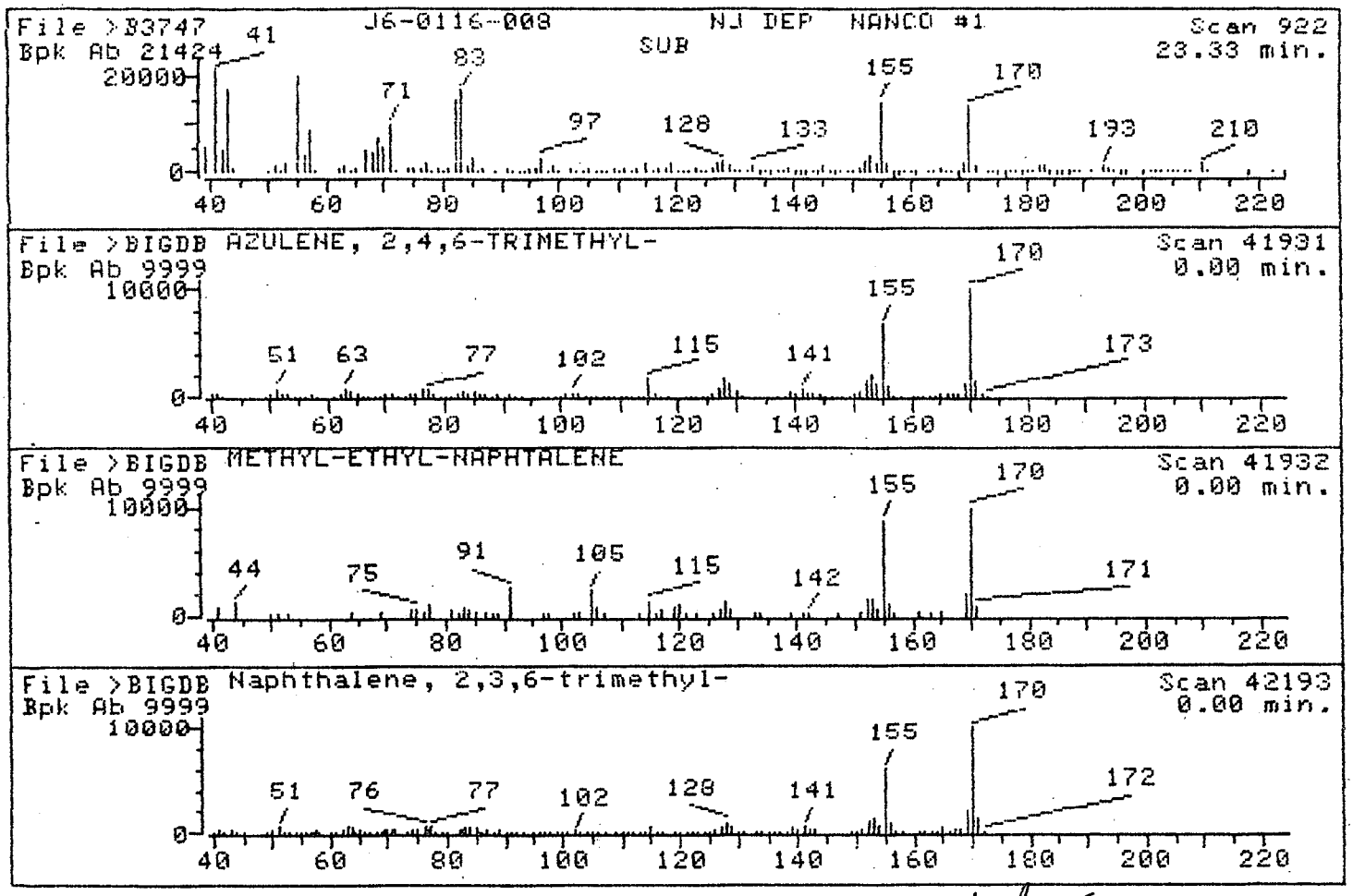


000280

1. Decane	142	C10H22
2. Decane	142	C10H22
3. Hexane, 4-ethyl-2-methyl-	128	C9H20
4. Decane, 2,6,8-trimethyl-	184	C13H28
5. 2-Decene, 5-methyl-, (Z)-	154	C11H22

Sample file: >B3747 Spectrum #: 916
Search speed: 1 Tilting option: N No. of ion ranges searched: 47

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	67	124185	12668	"BIGDB	71	29	2	0	97	12	34	26
2.	67	124185	12670	"BIGDB	62	37	2	0	80	14	34	21
3.	63*	3074757	18571	"BIGDB	42	47	0	0	87	32	22	48
4.	62*	62108263	7482	"BIGDB	44	48	0	0	100	28	25	49
5.	59*	74645866	18103	"BIGDB	40	40	0	0	100	37	21	50



Isomer of naphthalene

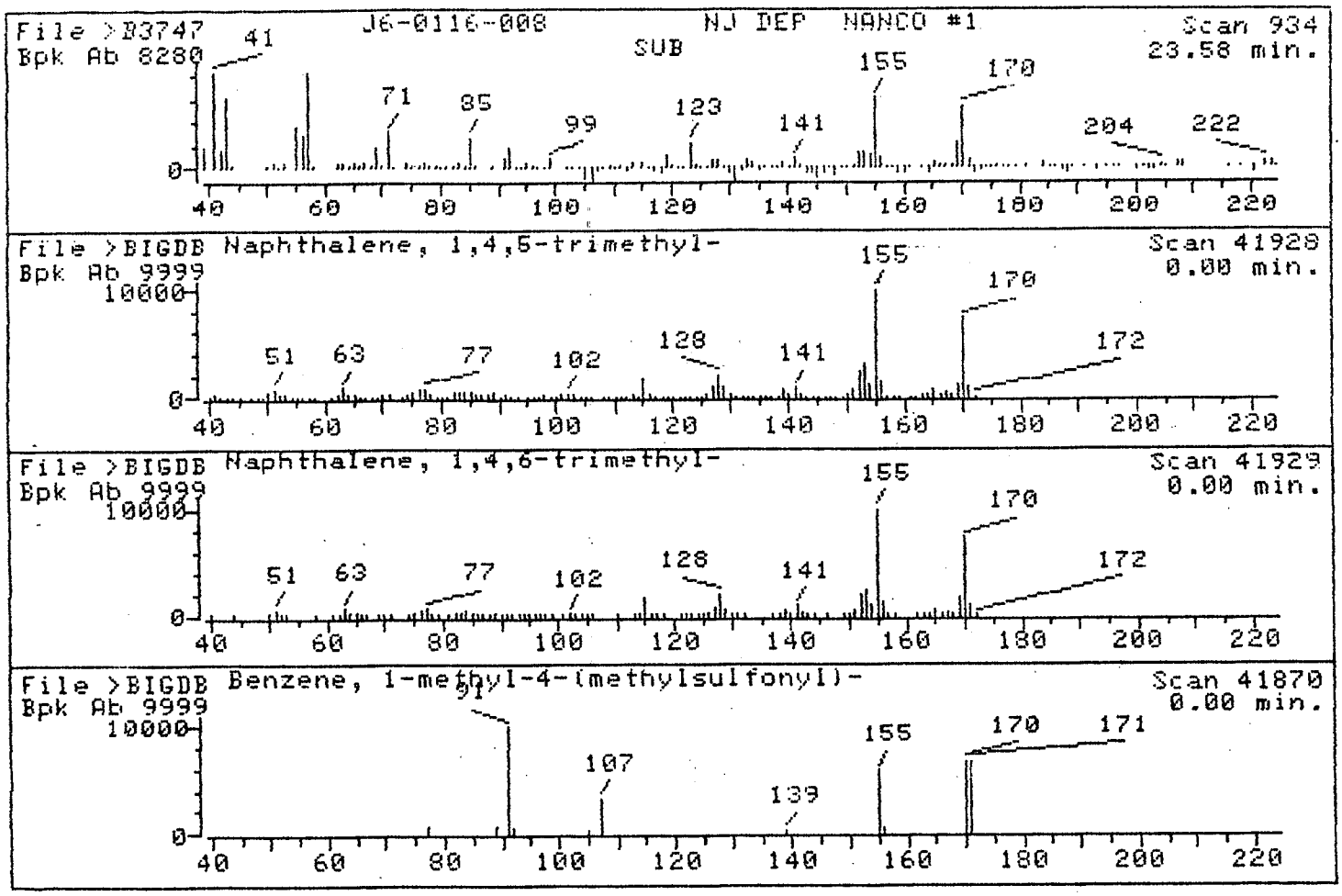
000281

16

1.	AZULENE, 2,4,6-TRIMETHYL-	170	C13H14
2.	METHYL-ETHYL-NAPHTALENE	170	C13H14
3.	Naphthalene, 2,3,6-trimethyl-	170	C13H14
4.	Naphthalene, 1,6,7-trimethyl-	170	C13H14
5.	Naphthalene, 1,4,6-trimethyl-	170	C13H14

Sample file: >B3747 Spectrum #: 922
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	26*	0	41931	"BIGDB	72	42	2	0	63	57	7	54
2.	23*	0	41932	"BIGDB	67	49	2	0	63	57	6	46
3.	21*	829265	42193	"BIGDB	61	48	2	0	63	57	5	38
4.	21*	2245387	41926	"BIGDB	60	48	2	0	63	57	5	37
5.	18*	2131422	41929	"BIGDB	88	31	2	0	50	64	5	67

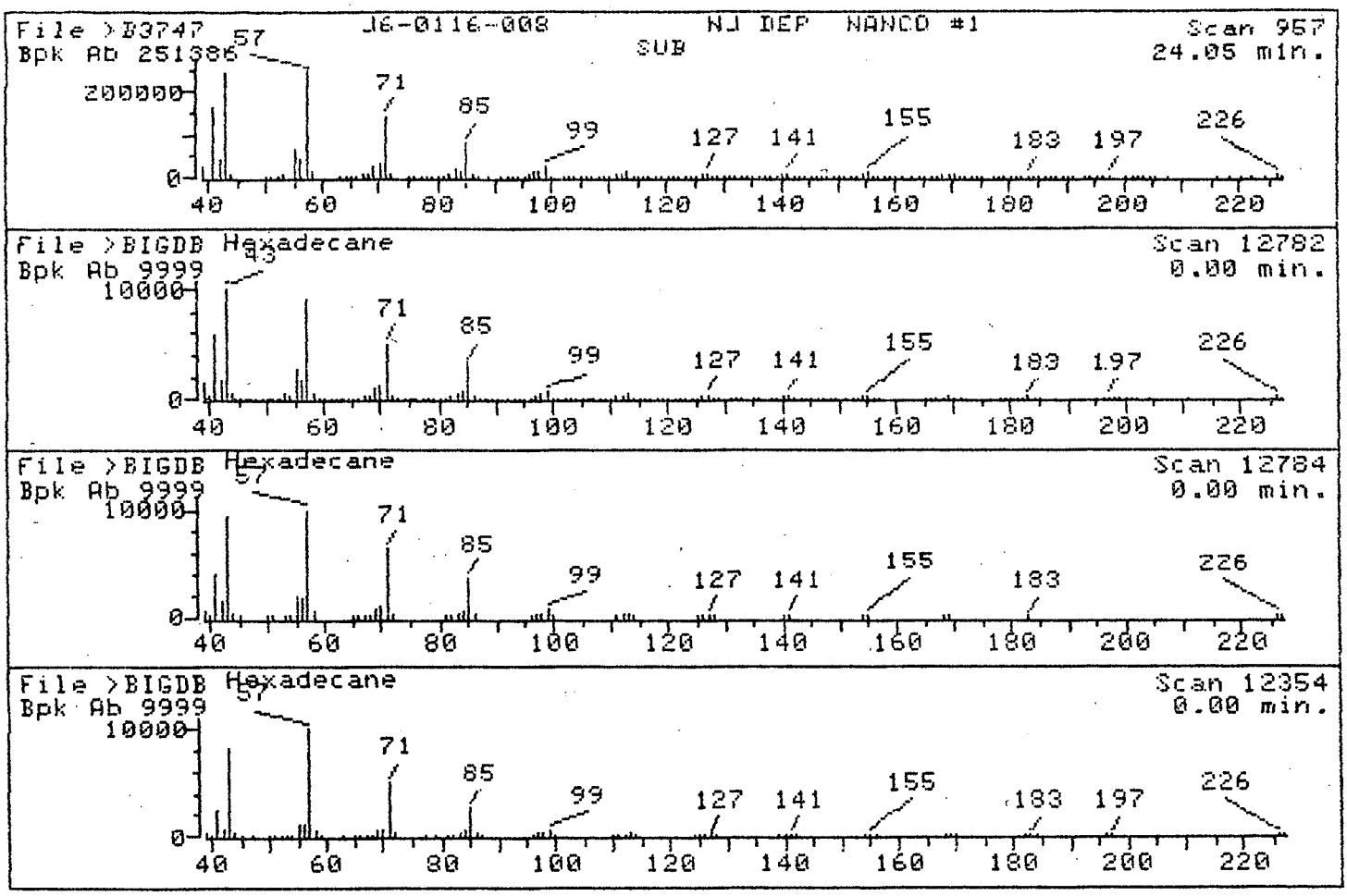


000282

1. Naphthalene, 1,4,5-trimethyl-	170	C13H14
2. Naphthalene, 1,4,6-trimethyl-	170	C13H14
3. Benzene, 1-methyl-4-(methylsulfonyl)-	170	C8H10O2S
4. METHYL-ETHYL-NAPHTALENE	170	C13H14
5. METHYL NAPTHYL KETONE(ORANGER)	170	C12H10O

Sample file: >B3747 Spectrum #: 934
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	44*	2131411	41928	"BIGDB	72	46	2	0	52	48	13	54
2.	40*	2131422	41929	"BIGDB	77	42	3	0	73	46	12	42
3.	25*	3185997	41870	"BIGDB	30	48	3	0	97	48	7	14
4.	25*	0	41932	"BIGDB	47	69	2	0	65	46	7	19
5.	25*	0	41923	"BIGDB	29	53	2	0	73	50	7	14

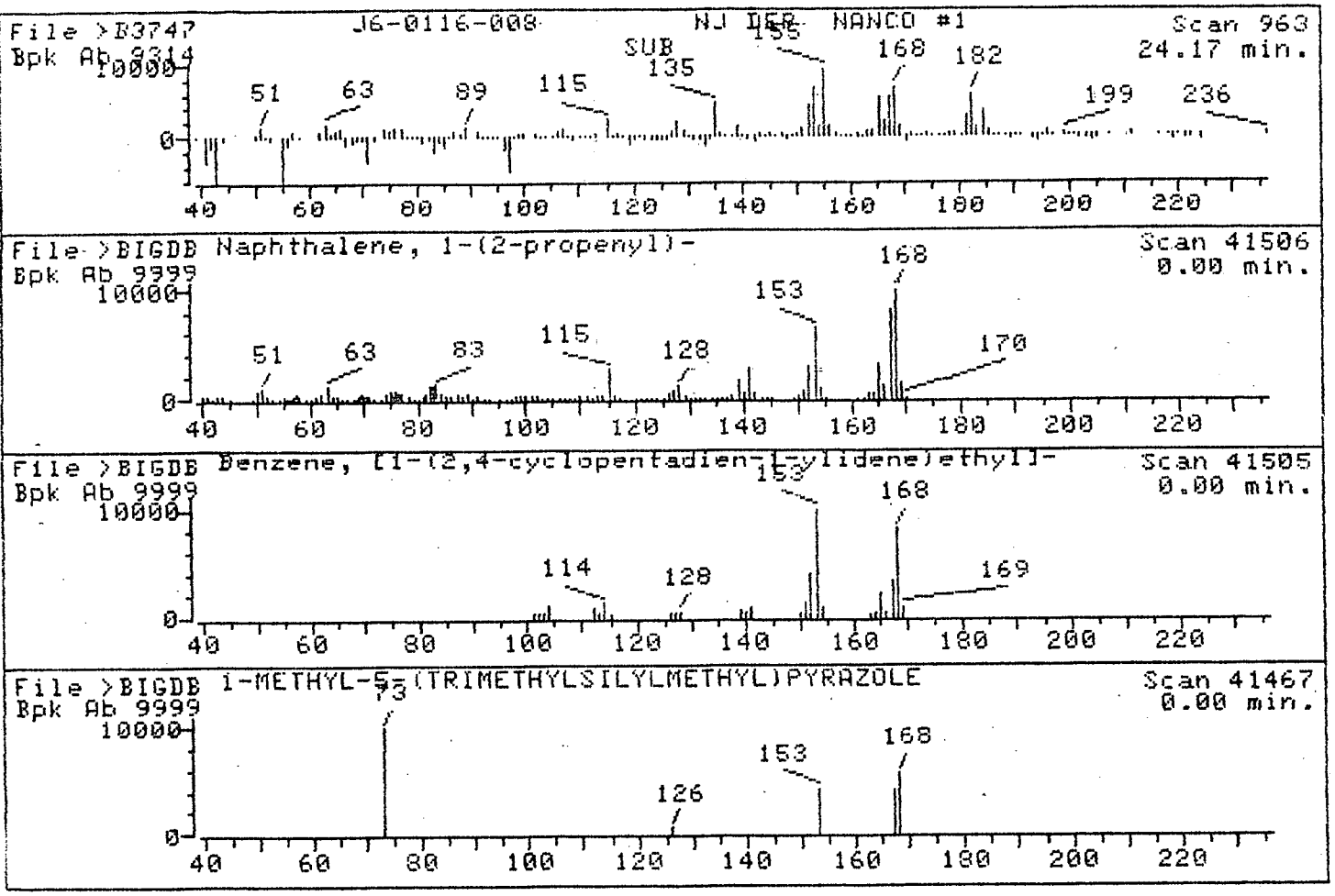


000283

1. Hexadecane	226	C16H34
2. Hexadecane	226	C16H34
3. Hexadecane	226	C16H34
4. Pentadecane	212	C15H32
5. Hexadecane	226	C16H34

Sample file: >B3747 Spectrum #: 957
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	99*	544763	12782	"BIGDB	115	1	0	0	87	4	72	99
2.	97*	544763	12784	"BIGDB	100	19	0	0	76	4	72	97
3.	96*	544763	12354	"BIGDB	82	25	0	0	90	2	72	94
4.	89	629629	12323	"BIGDB	104	8	1	0	80	4	66	76
5.	89	544763	12781	"BIGDB	106	13	1	0	73	4	66	67

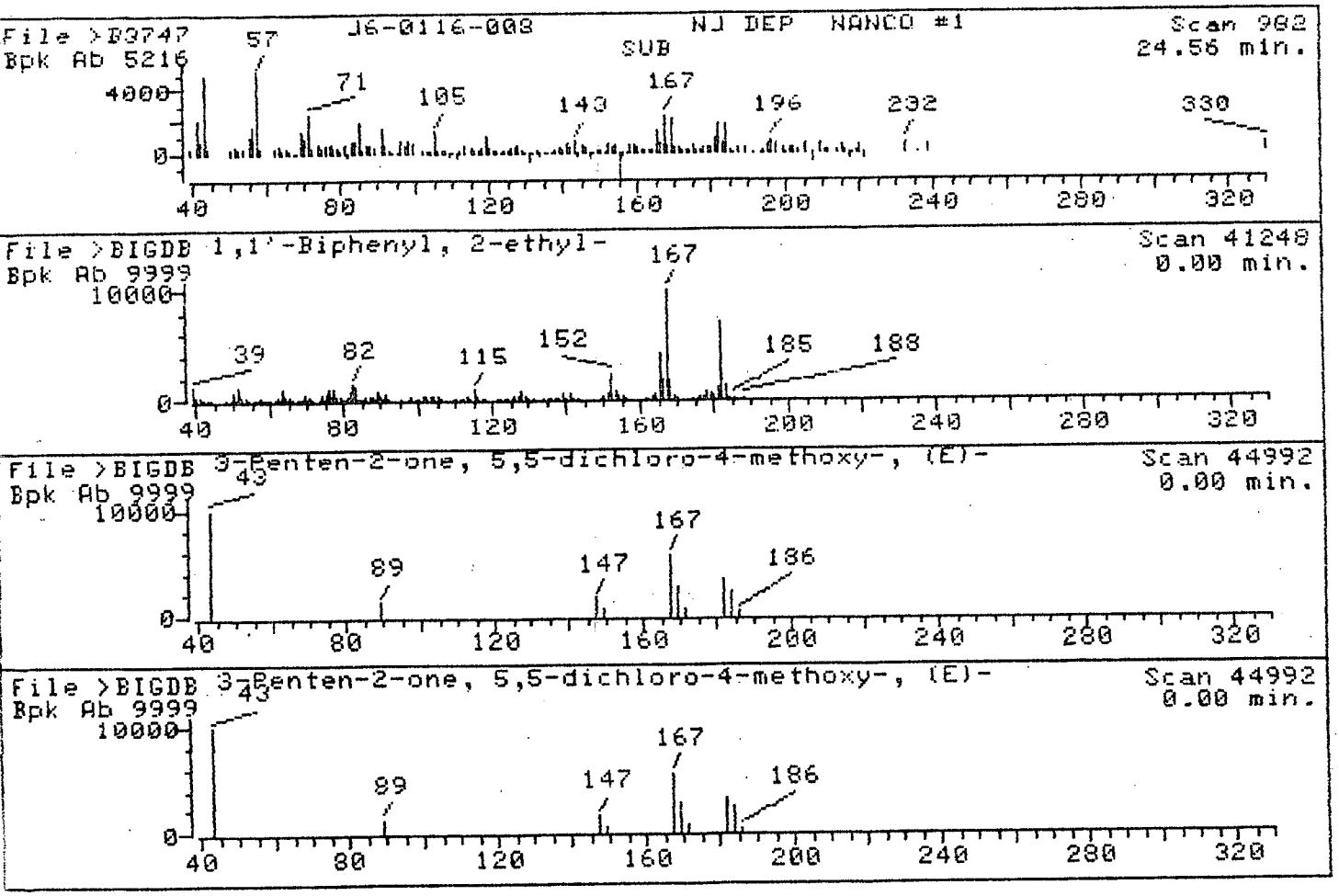


000284

1. Naphthalene, 1-(2-propenyl)- 168 C13H12
2. Benzene, [1-(2,4-cyclopentadien-1-ylidene)ethyl]- 168 C13H12
3. 1-METHYL-5-(TRIMETHYLSILYLMETHYL)PYRAZOLE 168 C8H16N2Si
4. 7,8-DIHYDRO-6H-BENZO(3,4)CYCLOBUTA(1,2)CYCLOHEPTENE 168 C13H12
5. Benzene, 1,1'-ethylidenebis- 182 C14H14

Sample file: >B3747 Spectrum #: 963
Search speed: 1 Tilting option: N No. of ion ranges searched: 47

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	18*	2489863	41506	"BIGDB	42	79	1	0	70	59	4	21
2.	15*	2320323	41505	"BIGDB	33	80	2	0	74	56	3	14
3.	15*	0	41467	"BIGDB	27	15	2	0	131	57	3	14
4.	11*	0	41512	"BIGDB	26	37	1	0	93	63	2	14
5.	11*	612000	41406	"BIGDB	49	64	3	0	168	63	2	13

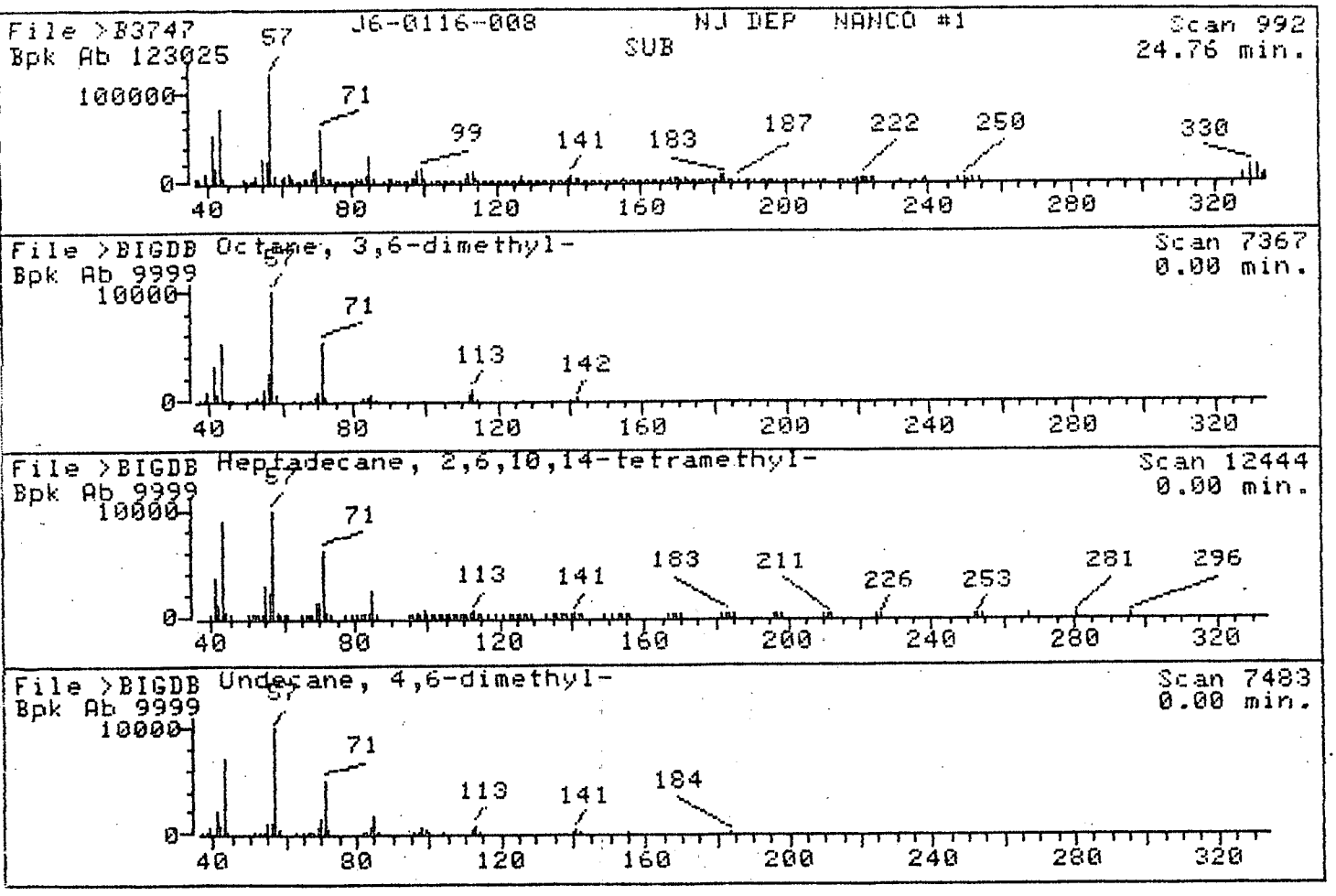


000285

1. 1,1'-Biphenyl, 2-ethyl- 182 C14H14
2. 3-Penten-2-one, 5,5-dichloro-4-methoxy-, (E)- 182 C6H8Cl2O2

Sample file: >B3747 Spectrum #: 982
Search speed: 1 Tilting option: N No. of ion ranges searched: 48

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	15*	1812517	41248	"BIGDB	72	37	1	0	43	66	5	71
2.	11*	61203756	44992	"BIGDB	23	53	2	0	77	62	2	13

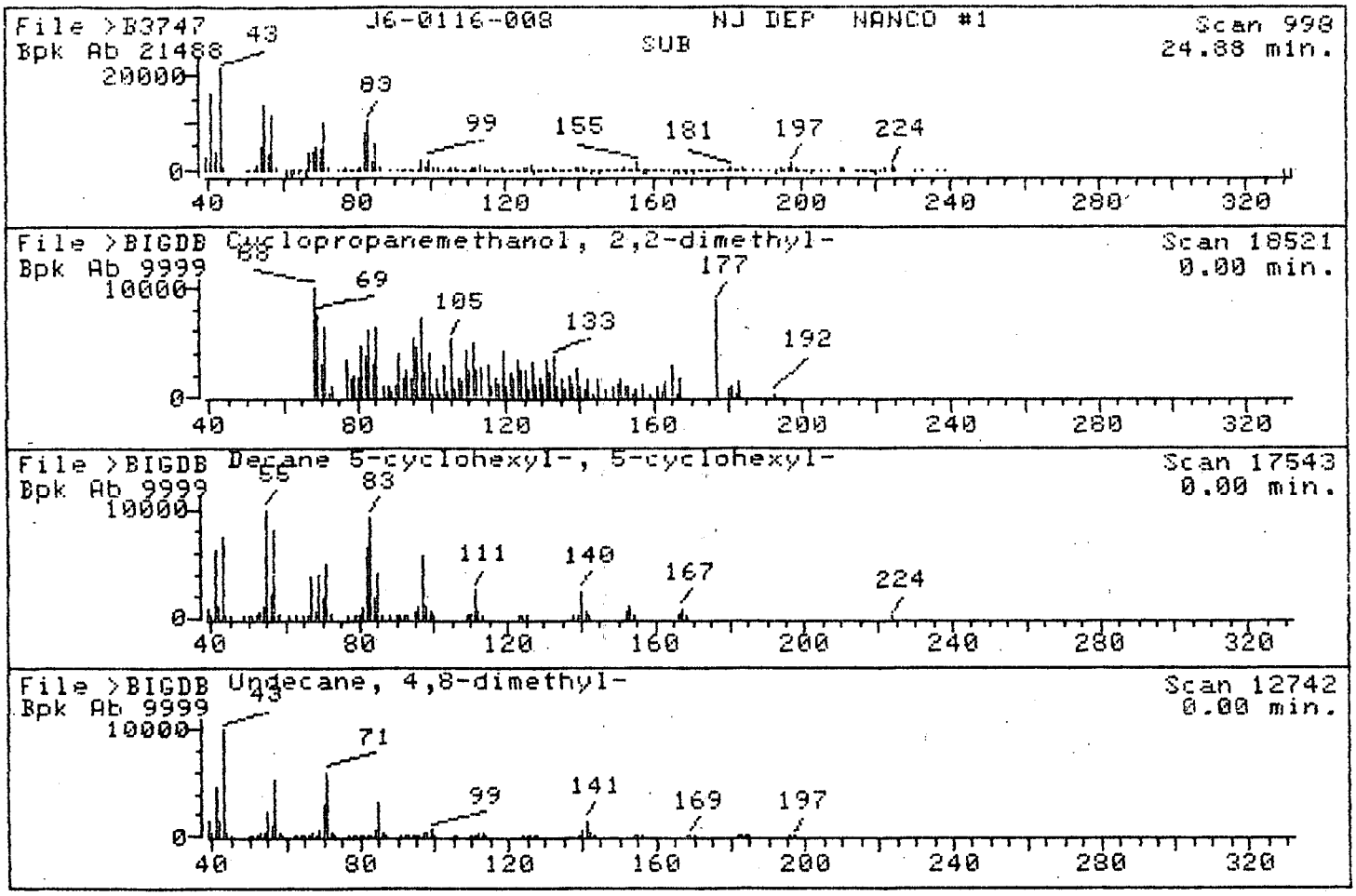


000286

1. Octane, 3,6-dimethyl- 142 C10H22
2. Heptadecane, 2,6,10,14-tetramethyl- 296 C21H44
3. Undecane, 4,6-dimethyl- 184 C13H28
4. PENTADECANE, 2,6,10-TRIMETHYL- (NOR-PRISTAN) 254 C18H38
5. Hexadecane 226 C16H34

Sample file: >B3747 Spectrum #: 992
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	69*	15869940	7367	"BIGDB	53	35	0	0	74	31	26	65
2.	59	18344371	12444	"BIGDB	79	46	1	0	66	23	27	31
3.	58	17312822	7483	"BIGDB	70	28	2	0	95	20	25	25
4.	57*	0	12398	"BIGDB	69	48	1	0	65	48	14	67
5.	55	544763	12354	"BIGDB	71	36	1	0	84	23	22	27



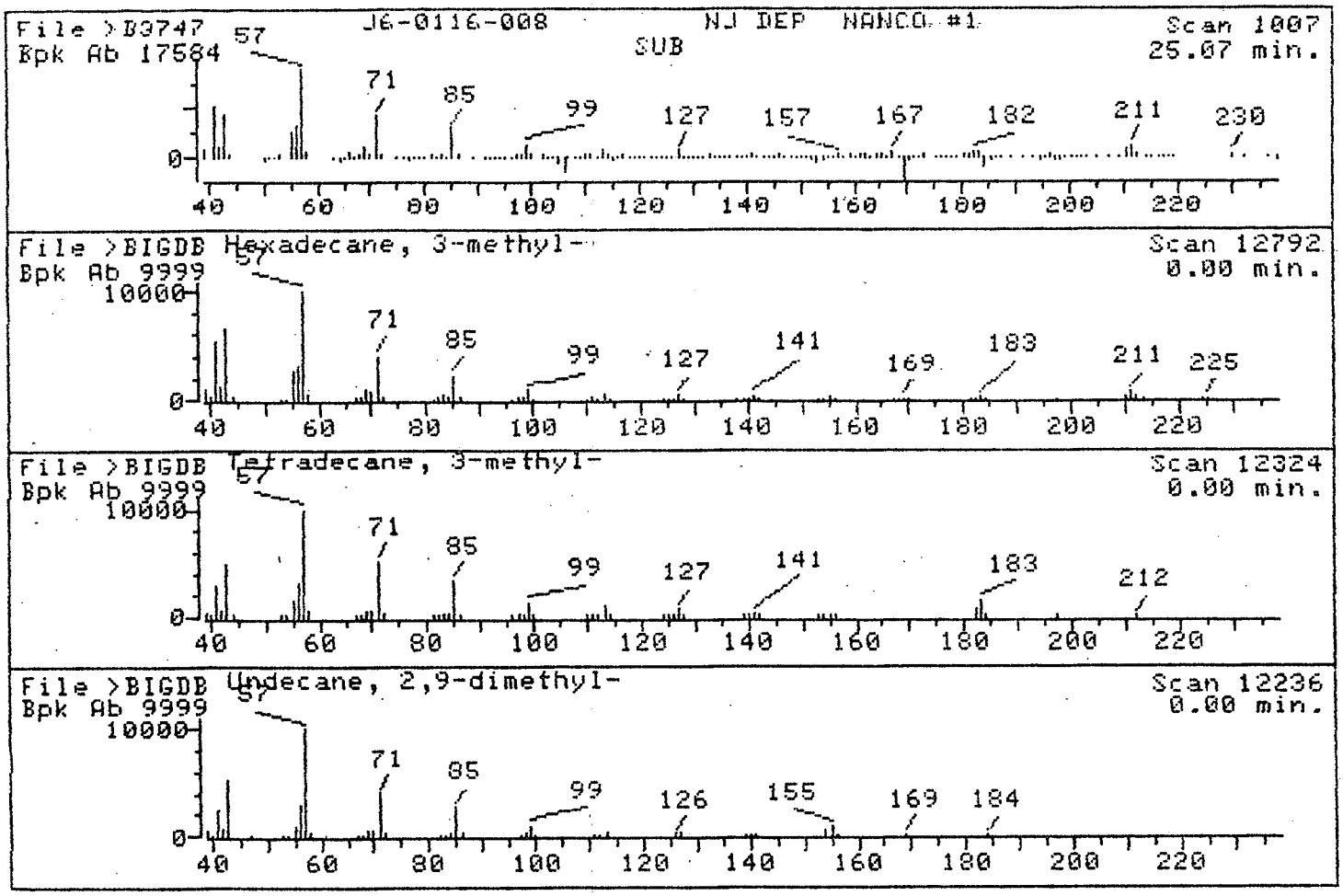
Unk

000287

1. Cyclopropanemethanol, 2,2-dimethyl-	100	C6H12O
2. Decane 5-cyclohexyl-, 5-cyclohexyl-	224	C16H32
3. Undecane, 4,8-dimethyl-	184	C13H28
4. Undecane, 3,8-dimethyl-	184	C13H28
5. DODECANE, 5-CYCLOHEXYL-	252	C18H36

Sample file: >B3747 Spectrum #: 998
Search speed: 1 Tilting option: N No. of ion ranges searched: 47

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	52*	930507	18521	"BIGDB	29	92	3	0	71	17	20	13
2.	31*	13151763	17543	"BIGDB	54	94	3	0	50	40	10	17
3.	28*	17301336	12742	"BIGDB	54	57	2	0	67	54	8	31
4.	28	17301303	12235	"BIGDB	63	45	0	0	50	54	8	31
5.	26	13151854	17589	"BIGDB	70	80	3	0	51	36	10	12

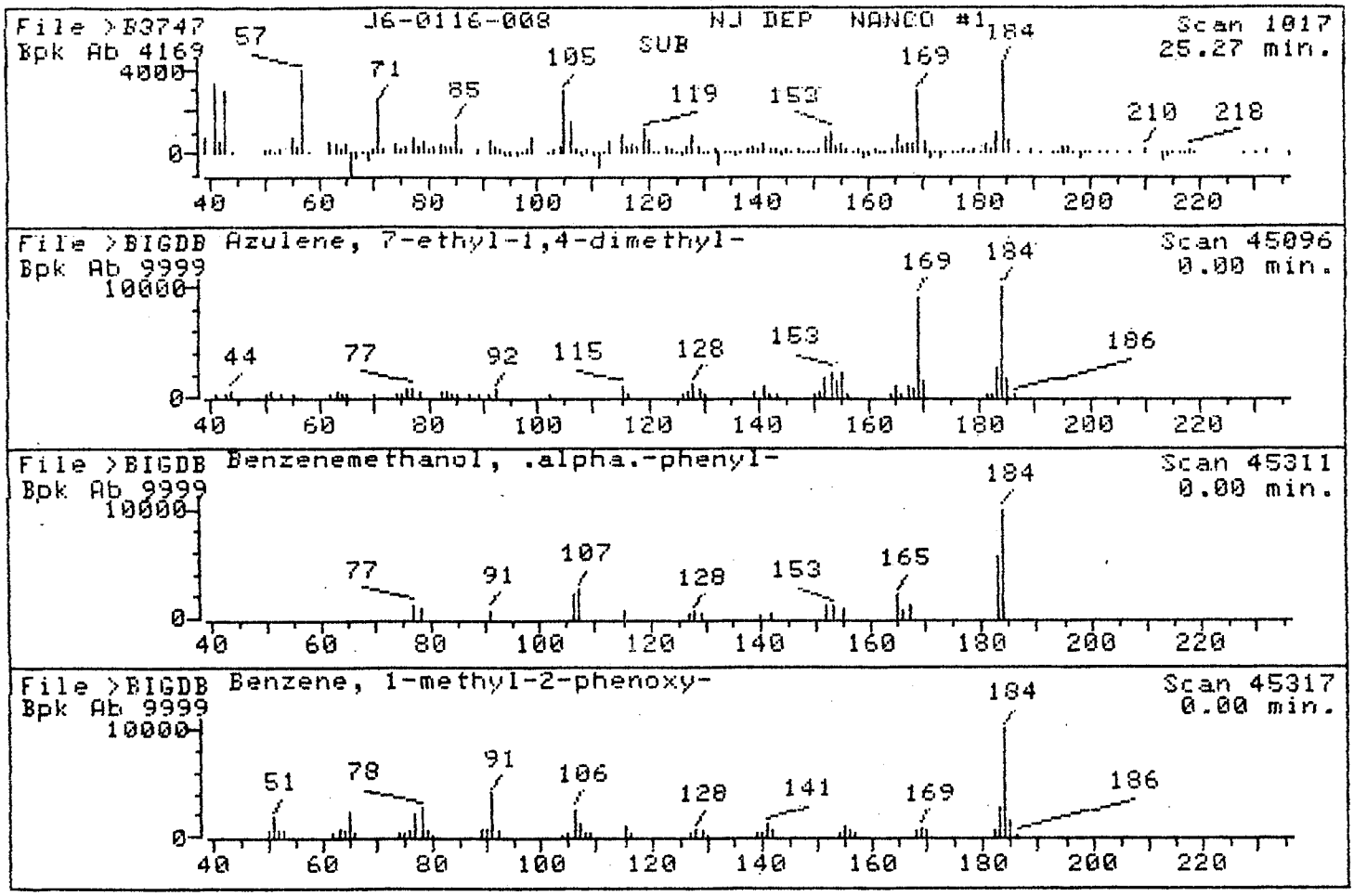


000288

1. Hexadecane, 3-methyl-	240	C17H36
2. Tetradecane, 3-methyl-	212	C15H32
3. Undecane, 2,9-dimethyl-	184	C13H28
4. Undecane, 3-methyl-	170	C12H26
5. Undecane, 3-methyl-	170	C12H26

Sample file: >B3747 Spectrum #: 1007
Search speed: 1 Tilting option: N No. of ion ranges searched: 46

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
*1.	76	6418435	12792	"BIGDB	79	34	2	0	97	6	45	24
2.	67*	18435228	12324	"BIGDB	50	63	2	0	90	11	34	23
3.	60	17301267	12236	"BIGDB	59	42	2	0	100	12	30	16
4.	60	1002433	12166	"BIGDB	46	42	2	0	96	15	30	15
5.	60	1002433	12724	"BIGDB	46	45	2	0	98	15	30	14

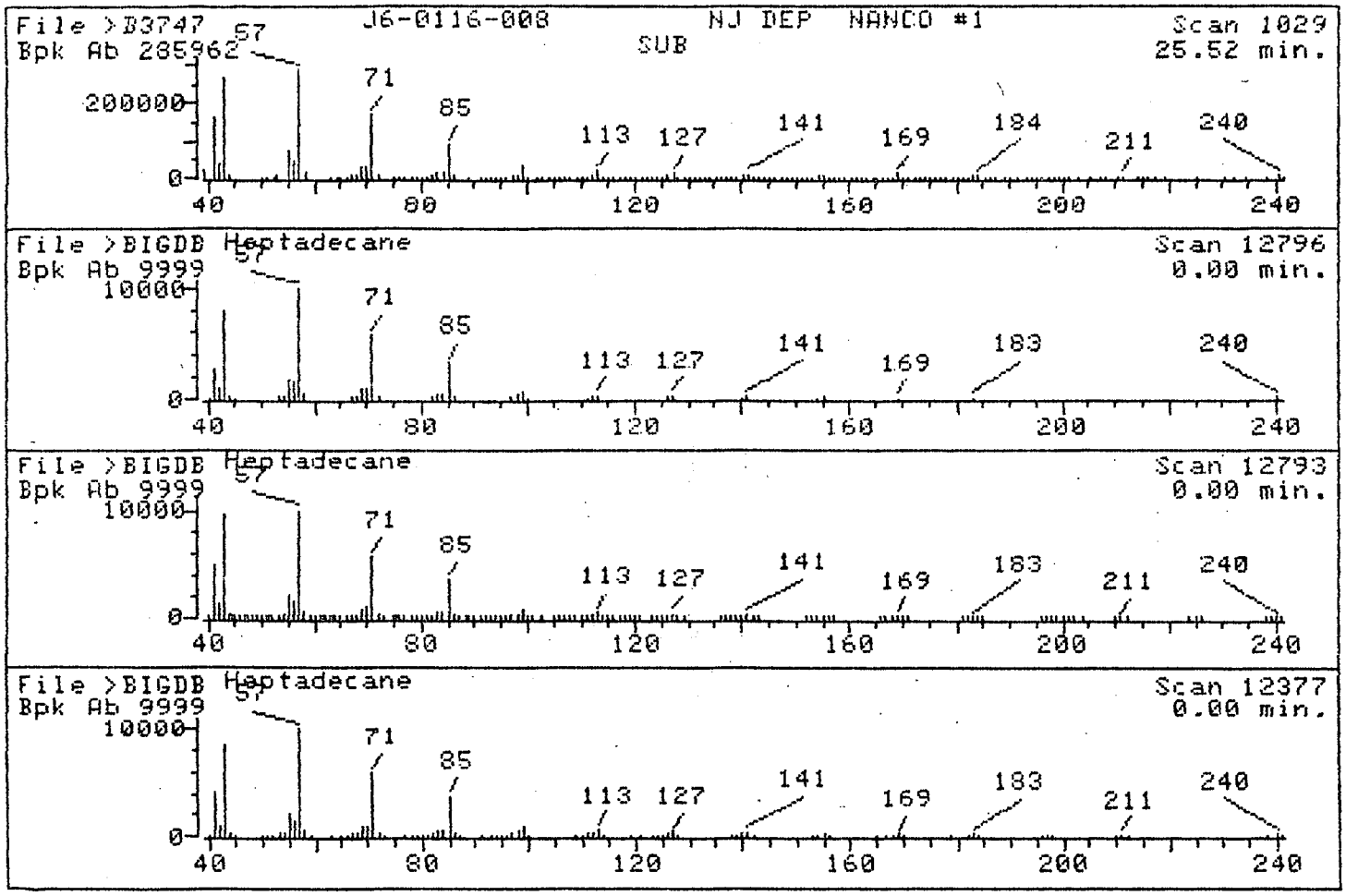


000289

1.	Azulene, 7-ethyl-1,4-dimethyl-	184 C14H16
2.	Benzenemethanol, .alpha.-phenyl-	184 C13H12O
3.	Benzene, 1-methyl-2-phenoxy-	184 C13H12O
4.	Benzene, 1-methyl-2-phenoxy-	184 C13H12O
5.	METHYL DIPHENYL ETHER	184 C13H12O

Sample file: >B3747 Spectrum #: 1017
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	71*	529055	45096	"BIGDB	93	39	2	0	76	32	32	72
2.	35*	91010	45311	"BIGDB	54	69	2	0	96	50	11	31
3.	35*	3991615	45317	"BIGDB	54	73	2	0	77	50	11	31
4.	35*	3991615	45084	"BIGDB	68	51	3	0	100	46	11	35
5.	31*	0	45091	"BIGDB	49	33	3	0	100	42	12	22



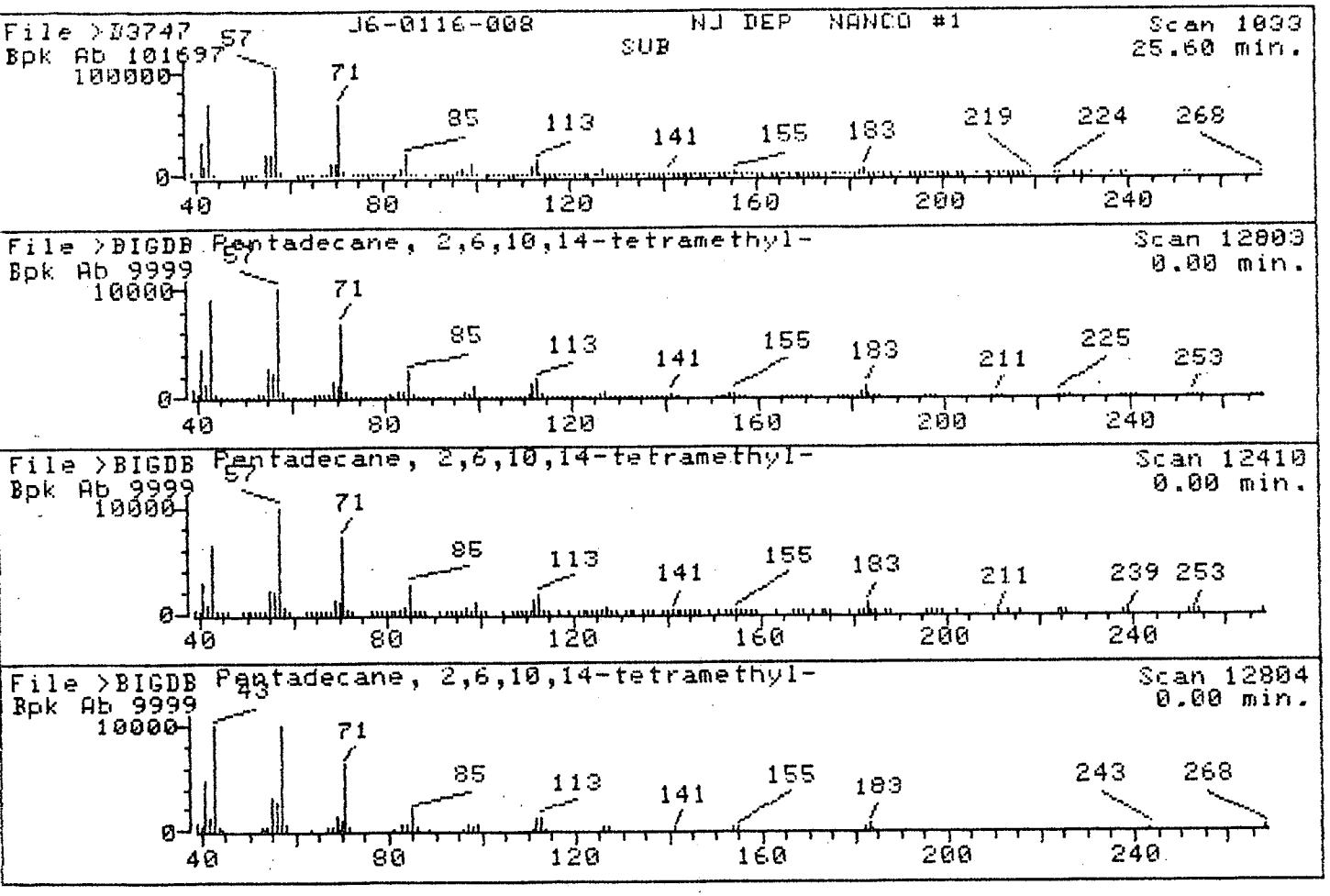
000290

J6

1. Heptadecane	240	C17H36
2. Heptadecane	240	C17H36
3. Heptadecane	240	C17H36
4. Tridecane	184	C13H28
5. Tridecane	184	C13H28

Sample file: >B3747 Spectrum #: 1029
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	97*	629787	12796	"BIGDB	95	16	0	0	95	5	72	97
2.	96*	629787	12793	"BIGDB	100	15	1	0	86	2	72	94
3.	96*	629787	12377	"BIGDB	88	34	0	0	72	2	72	96
4.	95*	629505	12748	"BIGDB	82	24	0	0	95	8	68	94
5.	89	629505	12750	"BIGDB	98	9	1	0	84	5	66	71



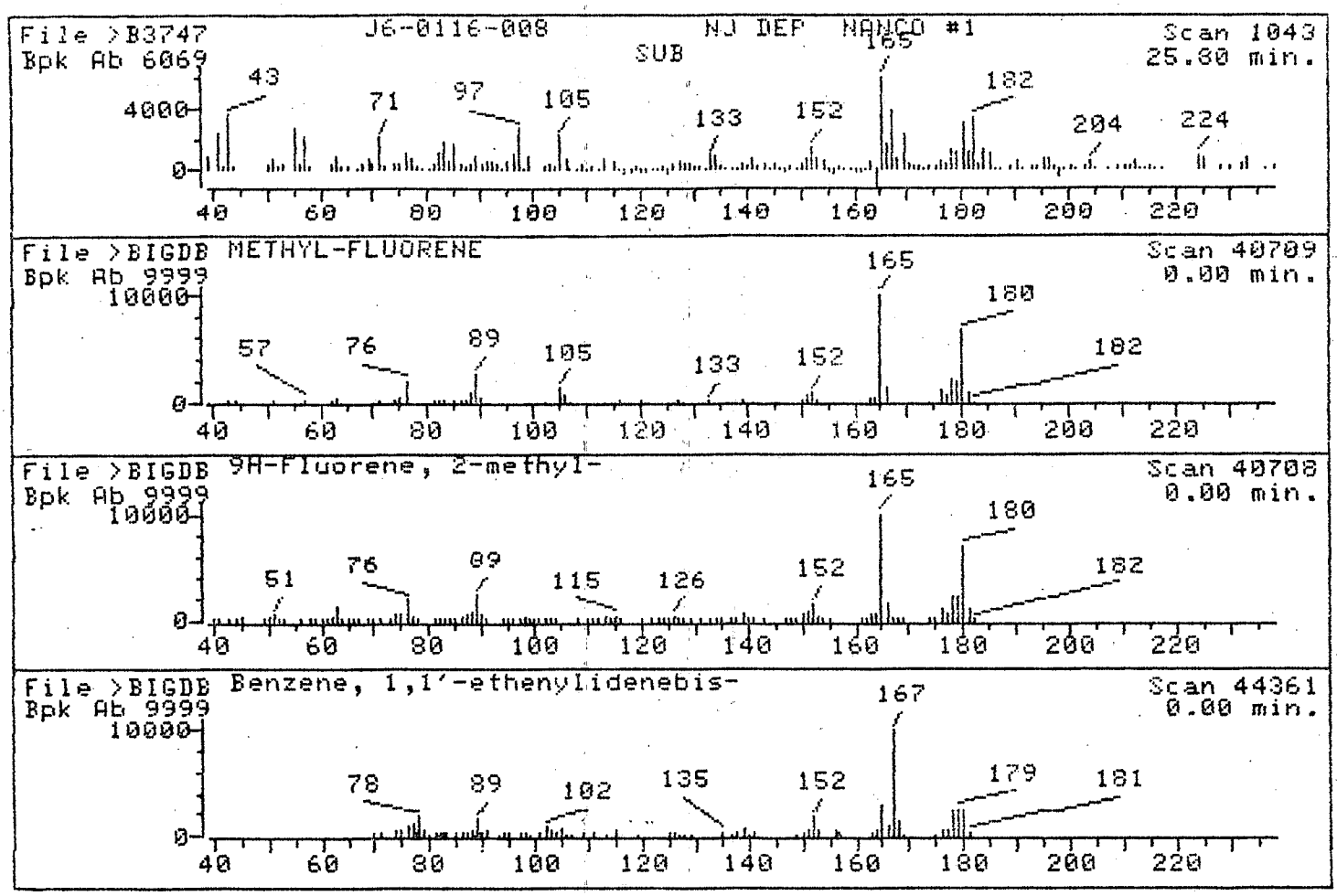
16

000291

1.	Pentadecane, 2,6,10,14-tetramethyl-	268 C19H40
2.	~~Pentadecane, 2,6,10,14-tetramethyl-~~	268 C19H40
3.	Pentadecane, 2,6,10,14-tetramethyl-	268 C19H40
4.	Dodecane, 2,7,10-trimethyl-	212 C15H32
5.	Dodecane, 2-methyl-8-propyl-	226 C16H34

Sample file: >B3747 Spectrum #: 1033
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	97*	1921706	12803	"BIGDB	118	12	1	0	72	0	72	97
2.	93*	1921706	12410	"BIGDB	106	26	2	0	70	0	68	83
3.	92*	1921706	12804	"BIGDB	86	44	0	0	63	28	57	95
4.	84	74645980	7540	"BIGDB	85	24	0	0	82	9	55	61
5.	83	55045073	12343	"BIGDB	82	46	2	0	67	1	57	22

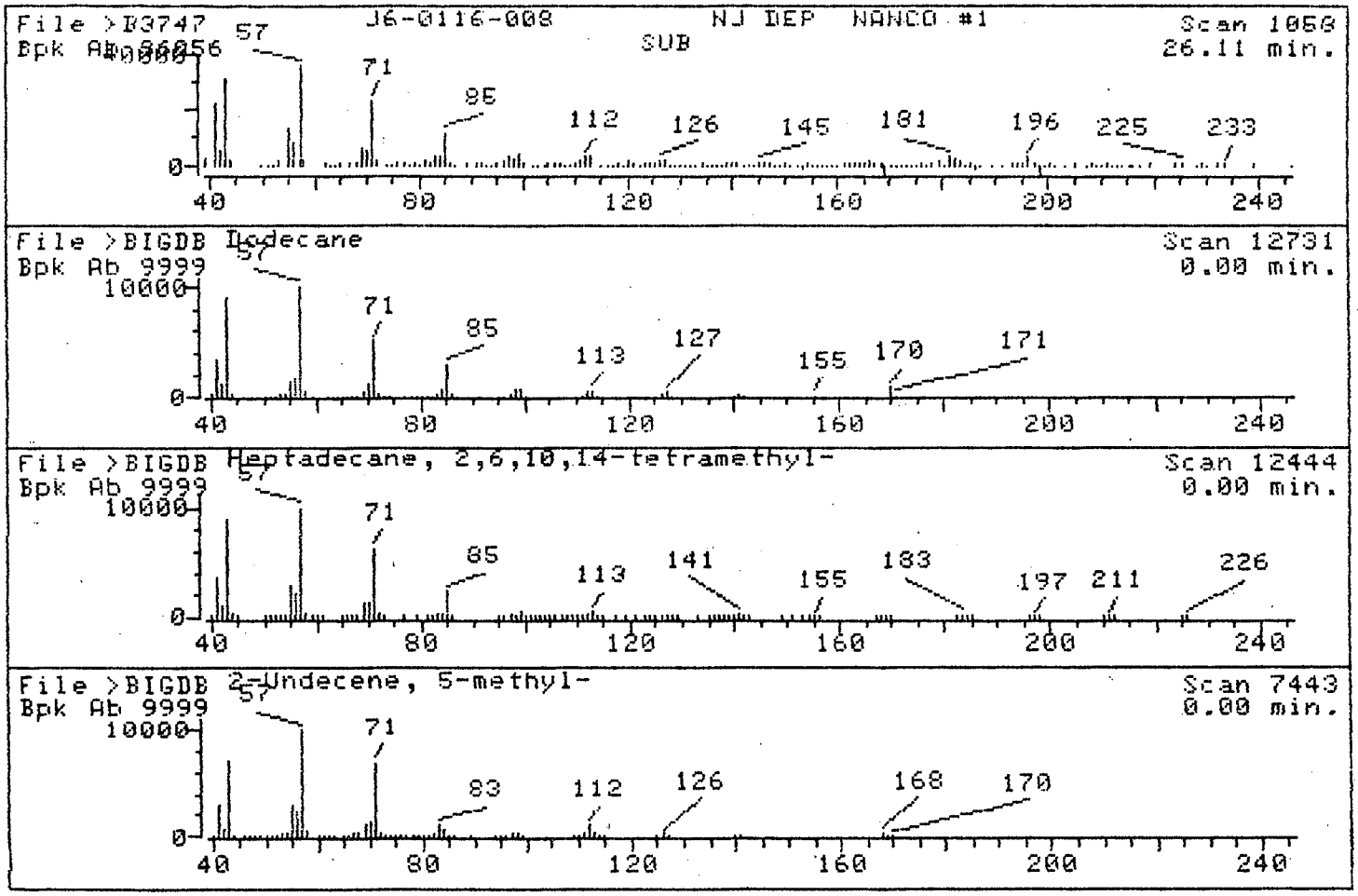


000292

1. METHYL-FLUORENE	180	C14H12
2. 9H-Fluorene, 2-methyl-	180	C14H12
3. Benzene, 1,1'-ethenylidenebis-	180	C14H12
4. 1,1'-Biphenyl, 2,4'-dimethyl-	182	C14H14
5. TERTIO BUTYL HYDROXY ANISOLE	180	C11H16O2

Sample file: >B3747 Spectrum #: 1043
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	28*	0	40709	"BIGDB	54	60	2	0	71	54	8	31
2.	28*	1430973	40708	"BIGDB	59	59	2	0	73	54	8	36
3.	20*	530483	44361	"BIGDB	28	117	3	0	66	53	5	13
4.	18*	611610	44679	"BIGDB	63	68	1	0	57	65	5	60
5.	15*	121006	40890	"BIGDB	36	70	3	0	80	60	3	13



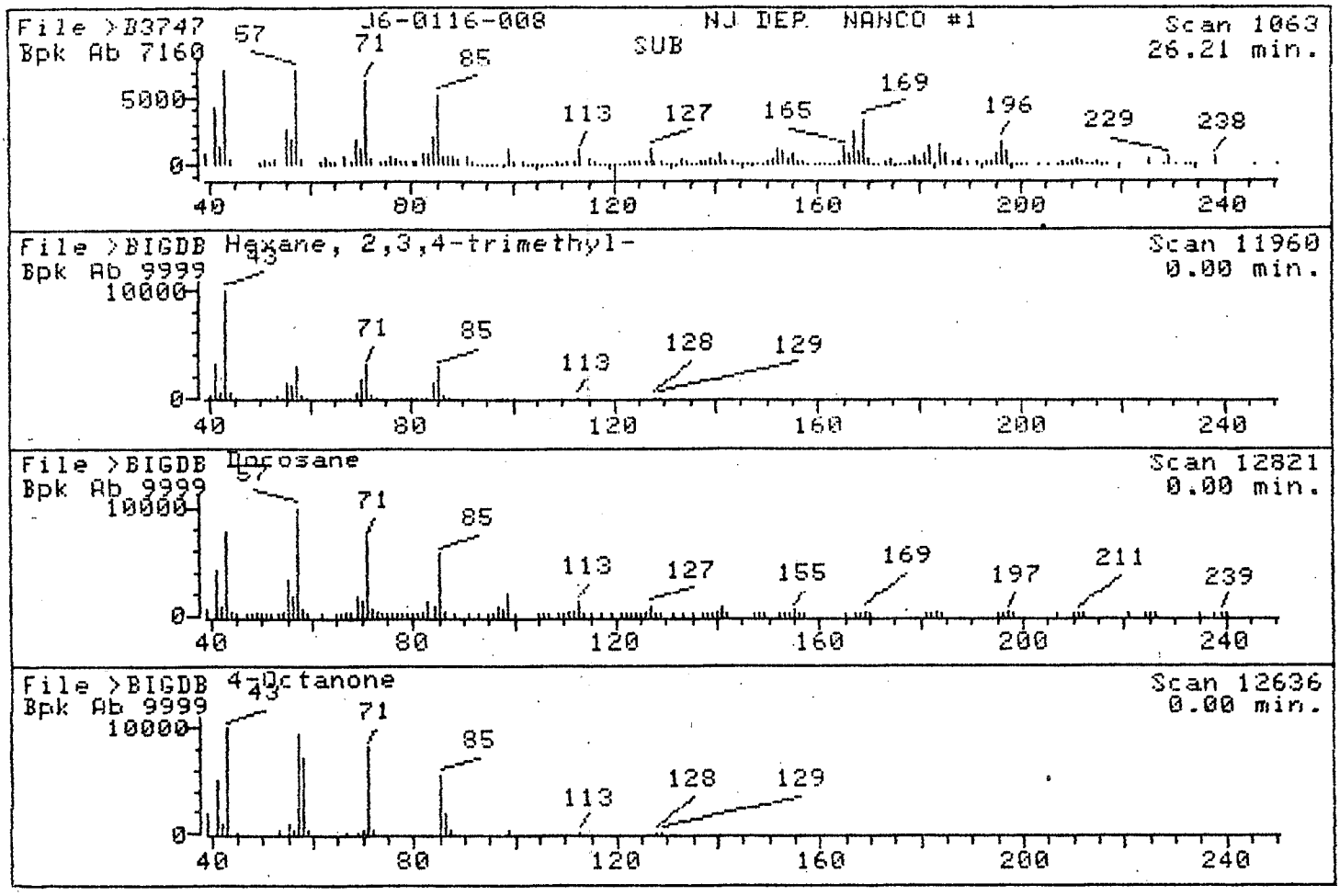
JM2 Hyd -16

000293

1.	Dodecane	170	C12H26
2.	Heptadecane, 2,6,10,14-tetramethyl-	296	C21H44
3.	2-Undecene, 5-methyl-	168	C12H24
4.	Dodecane	170	C12H26
5.	Tricosane	324	C23H48

Sample file: >B3747 Spectrum #: 1058
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	81	112403	12731	"BIGDB	81	18	1	0	94	8	53	42
2.	81	18344371	12444	"BIGDB	86	39	1	0	97	10	53	42
3.	81*	56851344	7443	"BIGDB	64	31	0	0	69	24	41	77
4.	79	112403	12730	"BIGDB	75	26	1	0	87	8	48	37
5.	76	638675	12470	"BIGDB	97	41	1	0	78	13	40	57

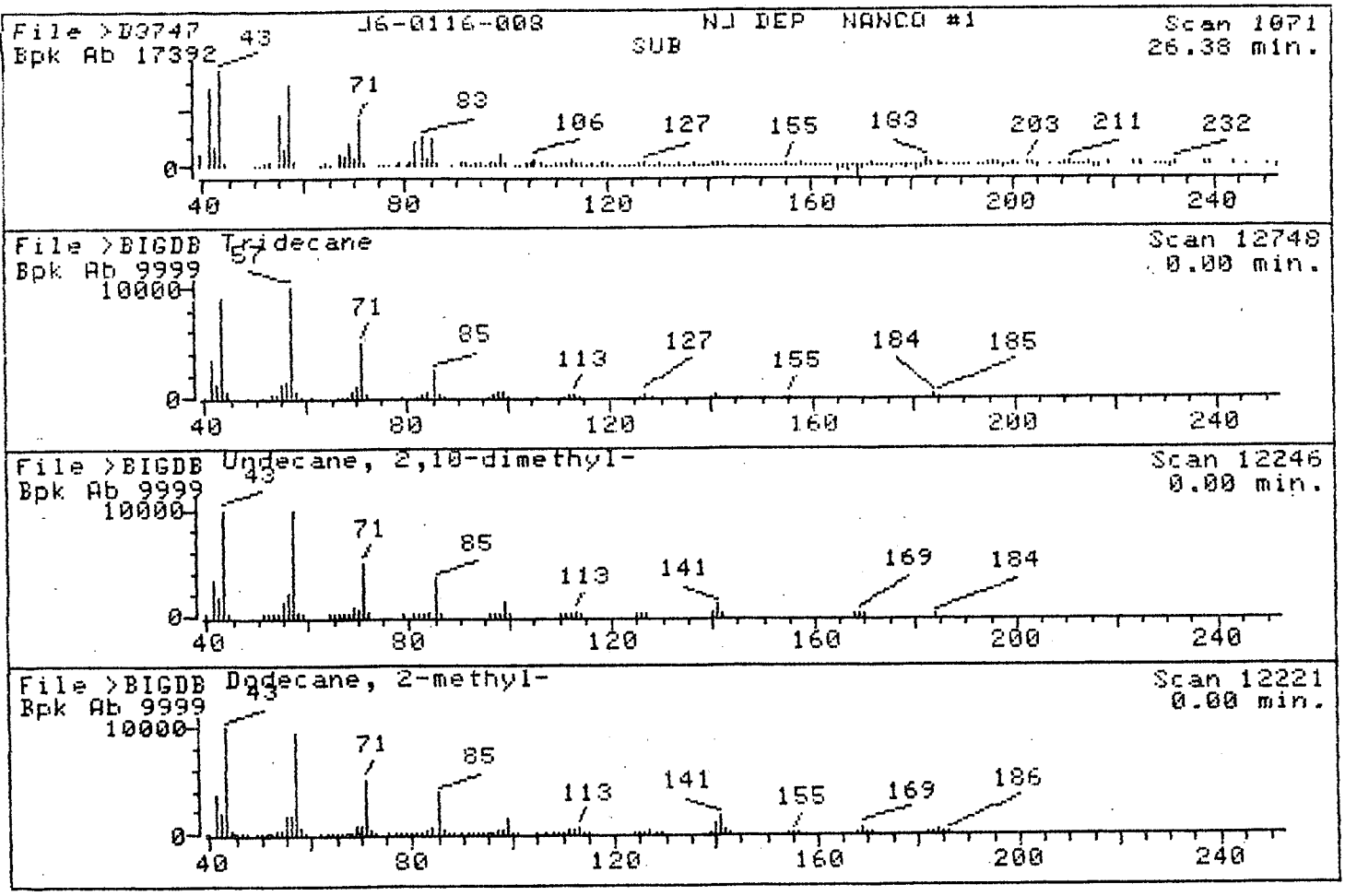


000294

1. Hexane, 2,3,4-trimethyl-	128	C9H20
2. Docosane	310	C22H46
3. 4-Octanone	128	C8H16O
4. Undecane, 2,7-dimethyl-	184	C13H28
5. Tridecane, 7-propyl-	226	C16H34

Sample file: >B3747 Spectrum #: 1063
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	41*	921471	11960	"BIGDB	48	42	2	0	210	40	14	28
2.	30	629970	12821	"BIGDB	73	74	2	0	86	44	8	18
3.	30*	589639	12636	"BIGDB	53	48	2	0	99	47	10	28
4.	27	17301245	12231	"BIGDB	52	47	2	0	155	40	10	13
5.	26	55045095	12351	"BIGDB	64	65	2	0	96	45	8	14

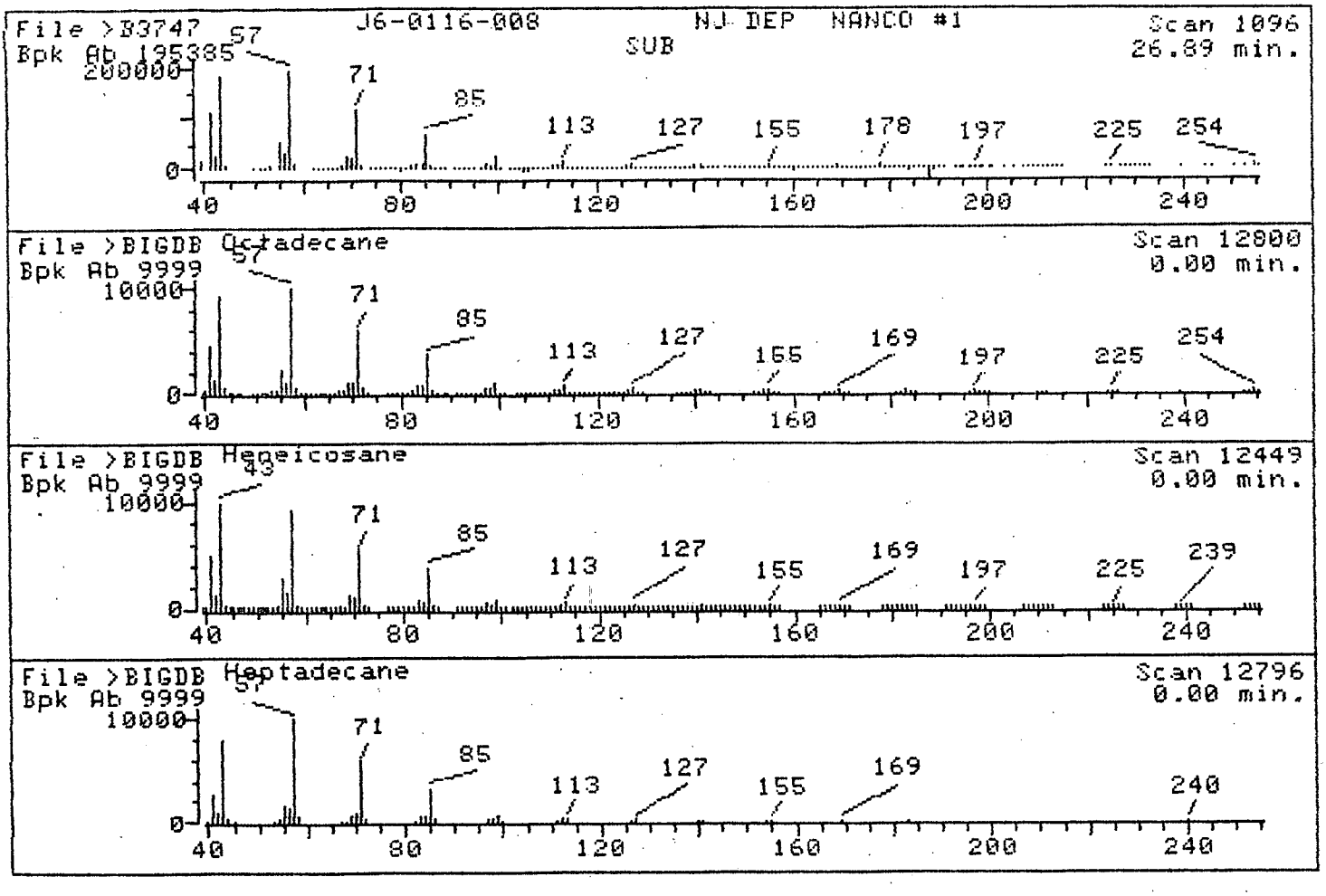


000295

1. Tridecane	184	C13H28
2. Undecane, 2,10-dimethyl-	184	C13H28
3. Dodecane, 2-methyl-	184	C13H28
4. Docosane, 7-hexyl-	394	C28H58
5. Tridecane, 2-methyl-	198	C14H30

Sample file: >B3747 Spectrum #: 1071
Search speed: 1 Tilting option: N No. of ion ranges searched: 45

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	65*	629505	12748	"BIGDB	60	46	1	0	83	32	24	56
2.	64*	17301278	12246	"BIGDB	64	45	2	0	79	21	28	43
3.	62*	1560970	12221	"BIGDB	69	46	2	0	71	26	25	49
4.	51	55373869	12515	"BIGDB	85	67	2	0	70	24	22	23
5.	49	1560969	12765	"BIGDB	74	37	2	0	83	21	22	21

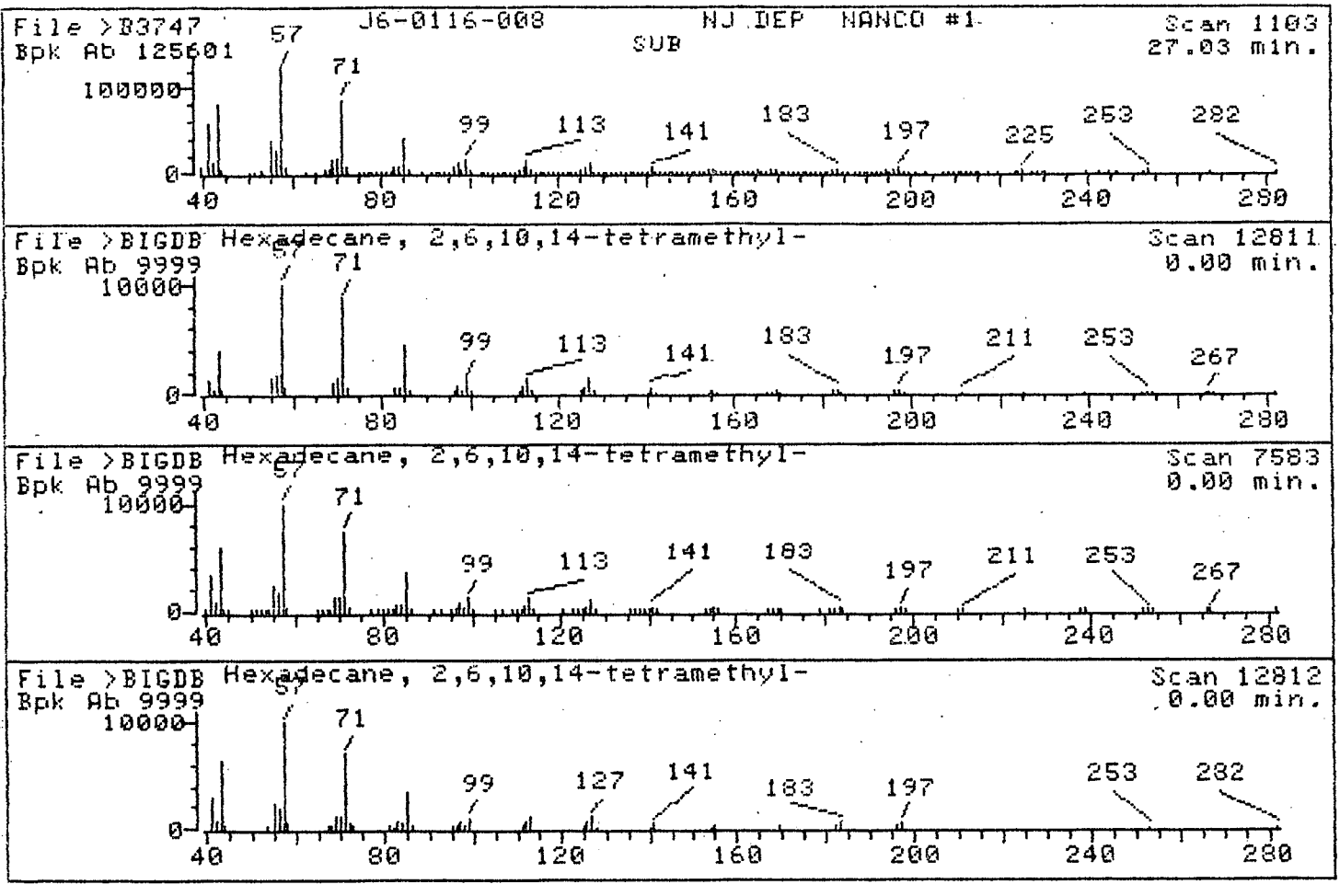


000296

1. Octadecane	254	C18H38
2. Heneicosane	296	C21H44
3. Heptadecane	240	C17H36
4. Heptadecane	240	C17H36
5. Pentadecane	212	C15H32

Sample file: >B3747 Spectrum #: 1096
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	96*	593453	12800	"BIGDB	113	12	1	0	78	2	72	96
2.	89	629947	12449	"BIGDB	108	19	1	0	73	4	66	66
3.	89	629787	12796	"BIGDB	96	15	1	0	100	5	66	63
4.	89	629787	12795	"BIGDB	101	20	1	0	74	4	66	60
5.	89	629629	12775	"BIGDB	92	14	1	0	100	5	66	61

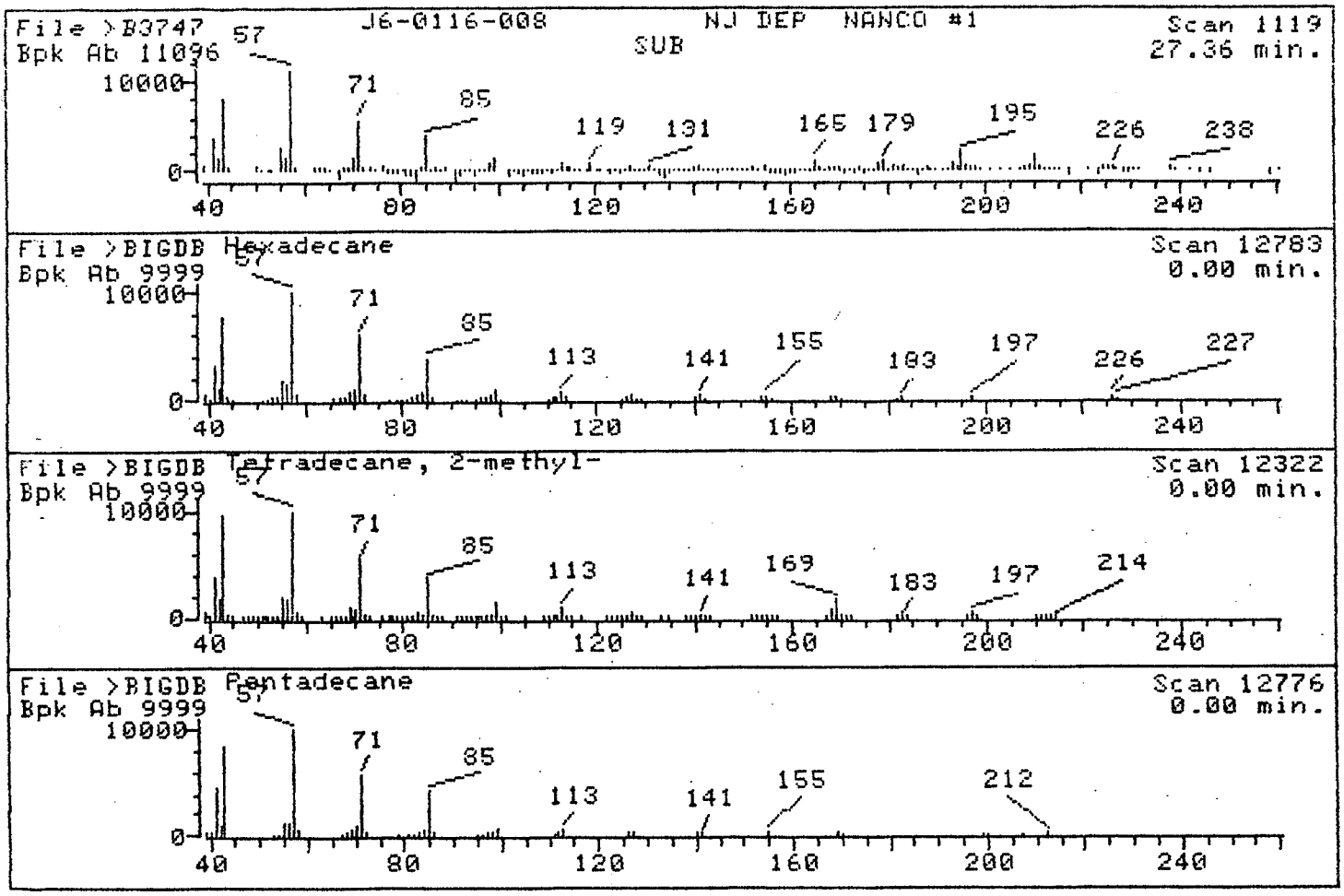


000297

1.	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42
2.	~~Hexadecane, 2,6,10,14-tetramethyl-~~	282 C20H42
3.	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42
4.	Tetracosane, 2,6,10,15,19,23-hexamethyl-	422 C30H62
5.	Dodecane, 2,6,10-trimethyl-	212 C15H32

Sample file: >B3747 Spectrum #: 1103
Search speed: 1 Tilting option: N No. of ion ranges searched: 46

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	96*	638368	12811	"BIGDB	112	21	1	0	68	4	72	96
2.	93*	638368	7583	"BIGDB	101	34	1	0	65	23	53	94
3.	83	638368	12812	"BIGDB	91	47	2	0	81	0	57	27
4.	83	111013	12853	"BIGDB	82	68	2	0	74	0	57	22
5.	81	3891983	12318	"BIGDB	72	34	0	0	88	8	53	49

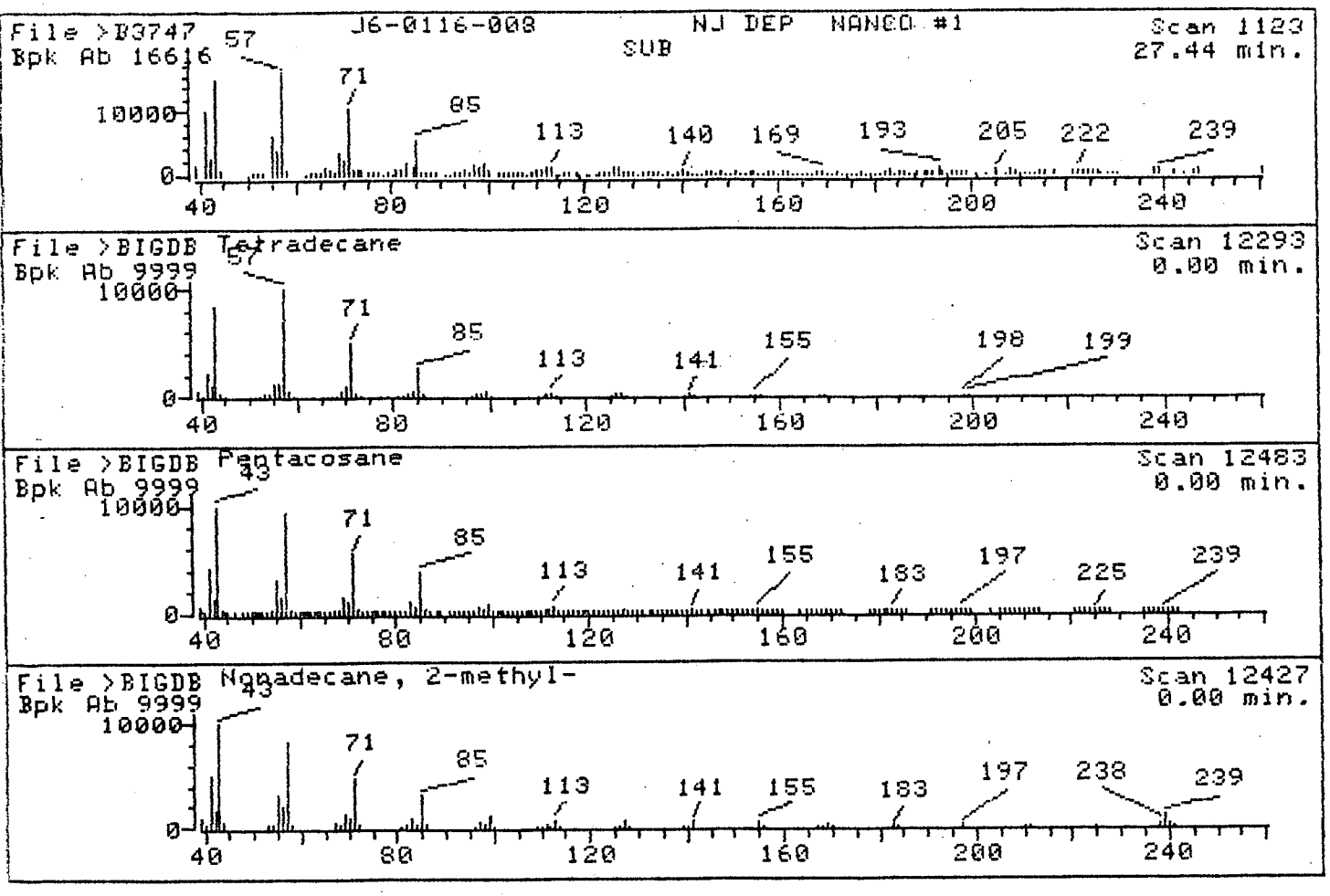


000298

1. Hexadecane	226	C16H34
2. Tetradecane, 2-methyl-	212	C15H32
3. Pentadecane	212	C15H32
4. Hexadecane	226	C16H34
5. Tetradecane	198	C14H30

Sample file: >B3747 Spectrum #: 1119
Search speed: 1 Tilting option: N No. of ion ranges searched: 53

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	85*	544763	12783	"BIGDB	87	33	0	0	76	50	40	95
2.	57*	1560958	12322	"BIGDB	89	35	2	0	74	48	14	67
3.	50*	629629	12776	"BIGDB	78	31	2	0	83	50	14	60
4.	49*	544763	12784	"BIGDB	62	57	0	0	73	52	16	74
5.	43*	629594	12770	"BIGDB	83	35	2	0	72	52	11	65

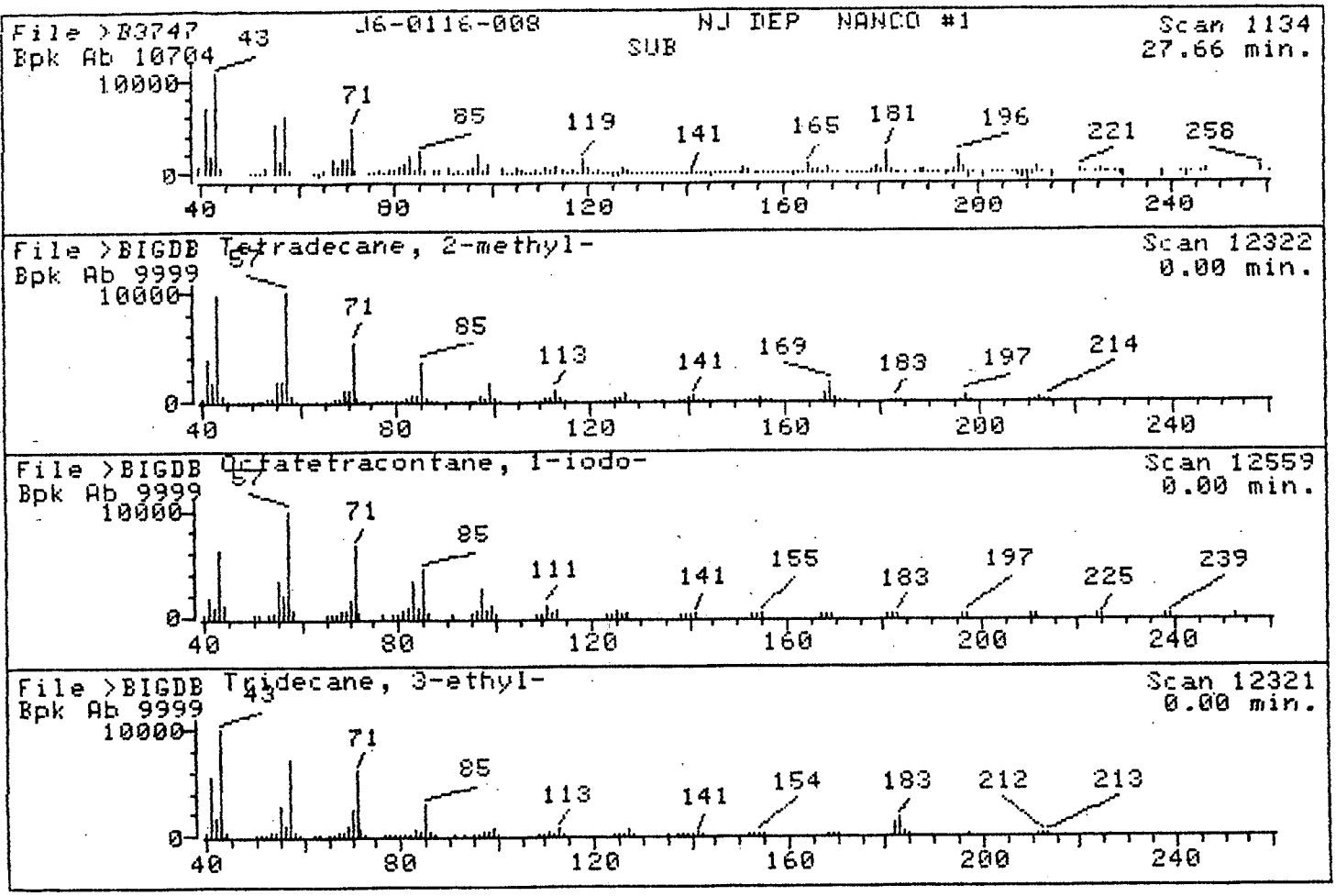


000299

1. Tetradecane — 198 C14H30
2. Pentacosane — 352 C25H52
3. Nonadecane, 2-methyl- — 282 C20H42
4. Heptadecane, 2-methyl- — 254 C18H38
5. Tricosane, 2-methyl- — 338 C24H50

Sample file: >B3747 Spectrum #: 1123
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	87*	629594	12293	"BIGDB	67	36	0	0	100	13	55	80
2.	79	629992	12483	"BIGDB	102	42	1	0	85	13	43	61
3.	78	1560867	12427	"BIGDB	61	75	2	0	87	4	55	12
4.	78	1560890	12395	"BIGDB	70	59	3	0	92	5	55	12
5.	76	1928309	12475	"BIGDB	95	46	2	0	89	6	45	29

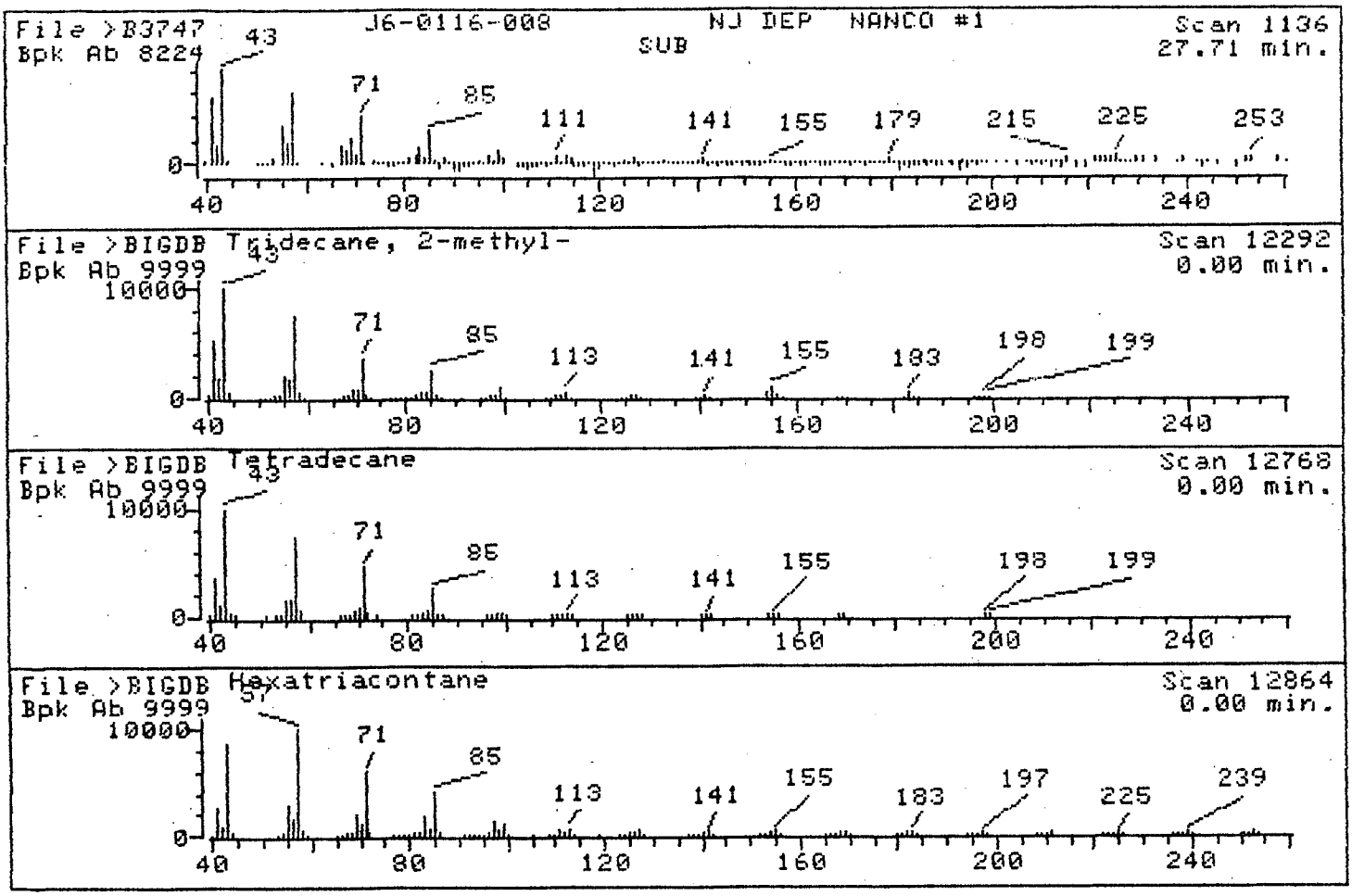


000300

1.	Tetradecane, 2-methyl-	212	C15H32
2.	Octatetracontane, 1-iodo-	800	C48H97I
3.	Tridecane, 3-ethyl-	212	C15H32
4.	Octadecane, 1-chloro-	288	C18H37Cl
5.	Triacontane, 11,20-didecyl-	702	C50H102

Sample file: >B3747 Spectrum #: 1134
Search speed: 1 Tilting option: N No. of ion ranges searched: 50

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	32*	1560958	12322	"BIGDB	68	56	2	0	55	53	9	49
2.	30	40710701	12559	"BIGDB	94	94	2	0	50	50	10	28
3.	28*	13286732	12321	"BIGDB	60	63	2	0	57	55	8	37
4.	25	3386332	12817	"BIGDB	63	77	2	0	53	48	7	13
5.	25	55256092	12865	"BIGDB	70	114	2	0	55	50	7	16

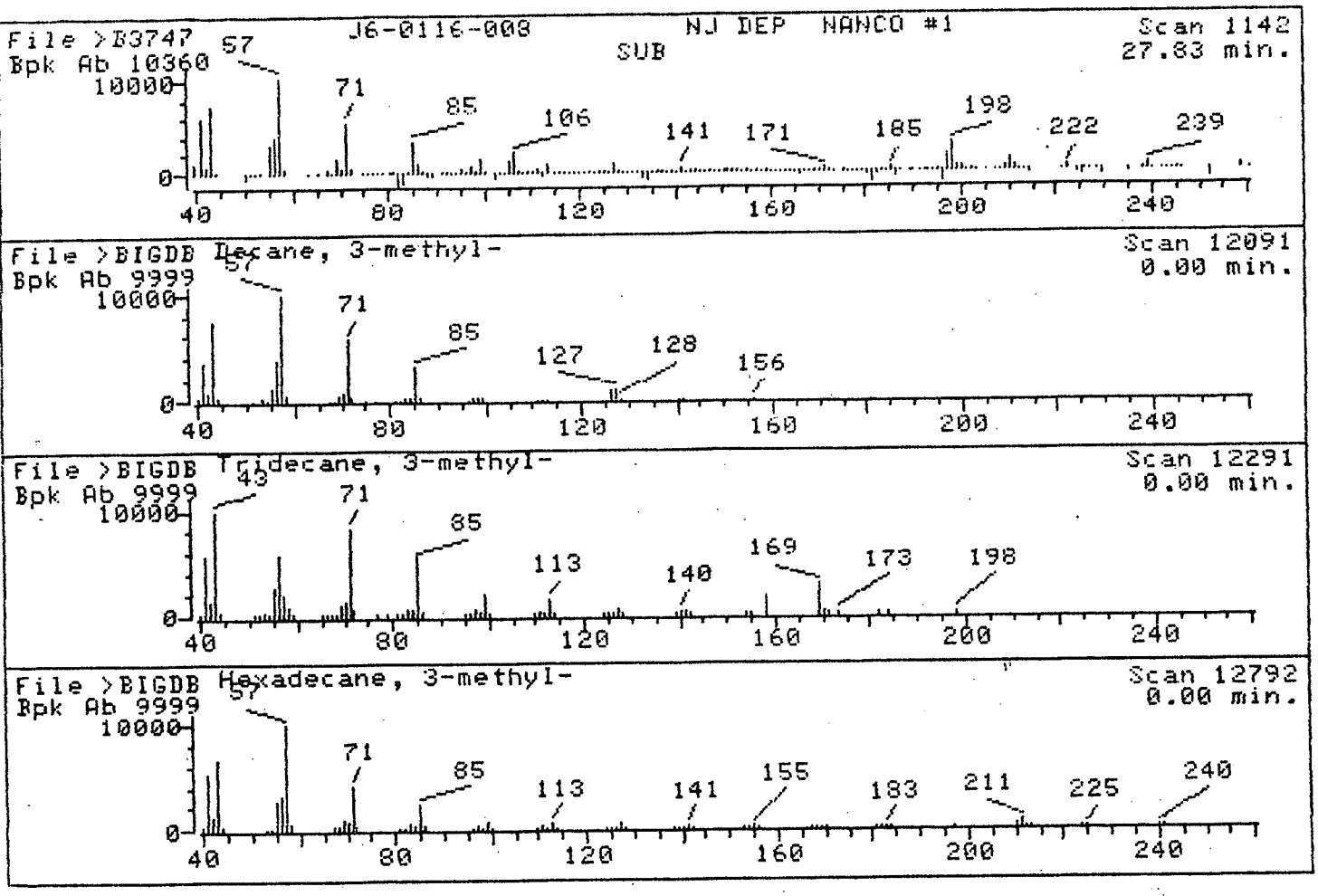


000301

1.	Tridecane, 2-methyl-	198 C14H30
2.	Tetradecane	198 C14H30
3.	Hexatriacontane	506 C36H74
4.	Tridecane, 2-methyl-	198 C14H30
5.	Eicosane, 2-methyl-	296 C21H44

Sample file: >B3747 Spectrum #: 1136
Search speed: 1 Tilting option: N No. of ion ranges searched: 53

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	54*	1560969	12292	"BIGDB	66	48	2	0	99	40	19	45
2.	53*	629594	12768	"BIGDB	56	52	1	0	98	40	19	44
3.	49	630068	12864	"BIGDB	100	62	2	0	72	35	20	33
4.	49*	1560969	12766	"BIGDB	62	58	2	0	74	40	19	40
5.	46	1560845	12447	"BIGDB	96	48	2	0	74	35	20	30

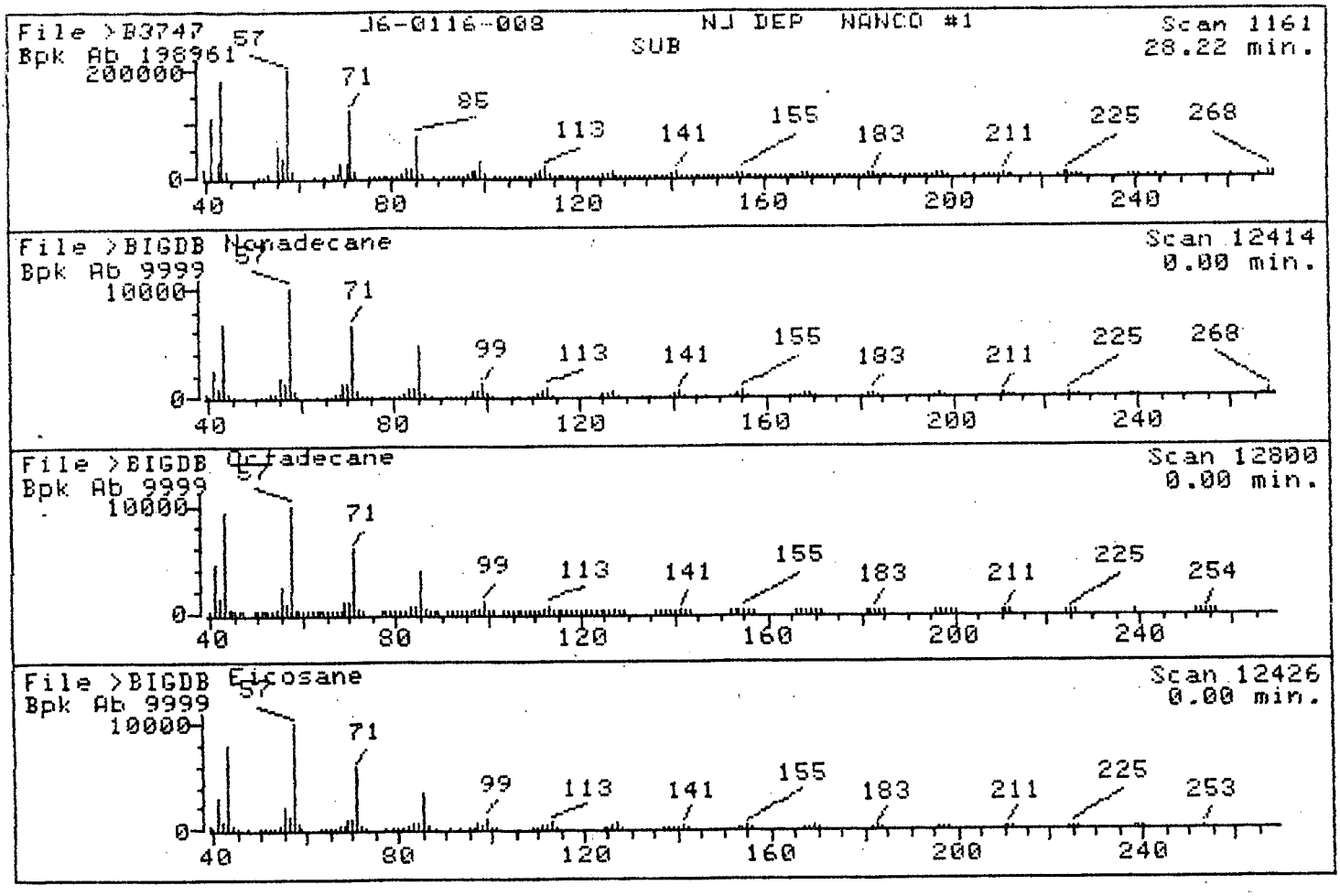


000302

1. Decane, 3-methyl- 156 C11H24
2. Tridecane, 3-methyl- 198 C14H30
3. Hexadecane, 3-methyl- 240 C17H36
4. Nonane, 3-methyl- 142 C10H22
5. Pentadecane, 3-methyl- 226 C16H34

Sample file: >B3747 Spectrum #: 1142
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	64*	13151343	12091	"BIGDB	70	24	1	0	82	42	18	69
2.	47*	6418413	12291	"BIGDB	62	66	2	0	60	41	16	40
3.	47*	6418435	12792	"BIGDB	68	45	2	0	100	41	16	49
4.	45*	5911046	7679	"BIGDB	63	23	1	0	100	52	11	67
5.	35	2882964	12349	"BIGDB	73	45	2	0	93	35	12	18



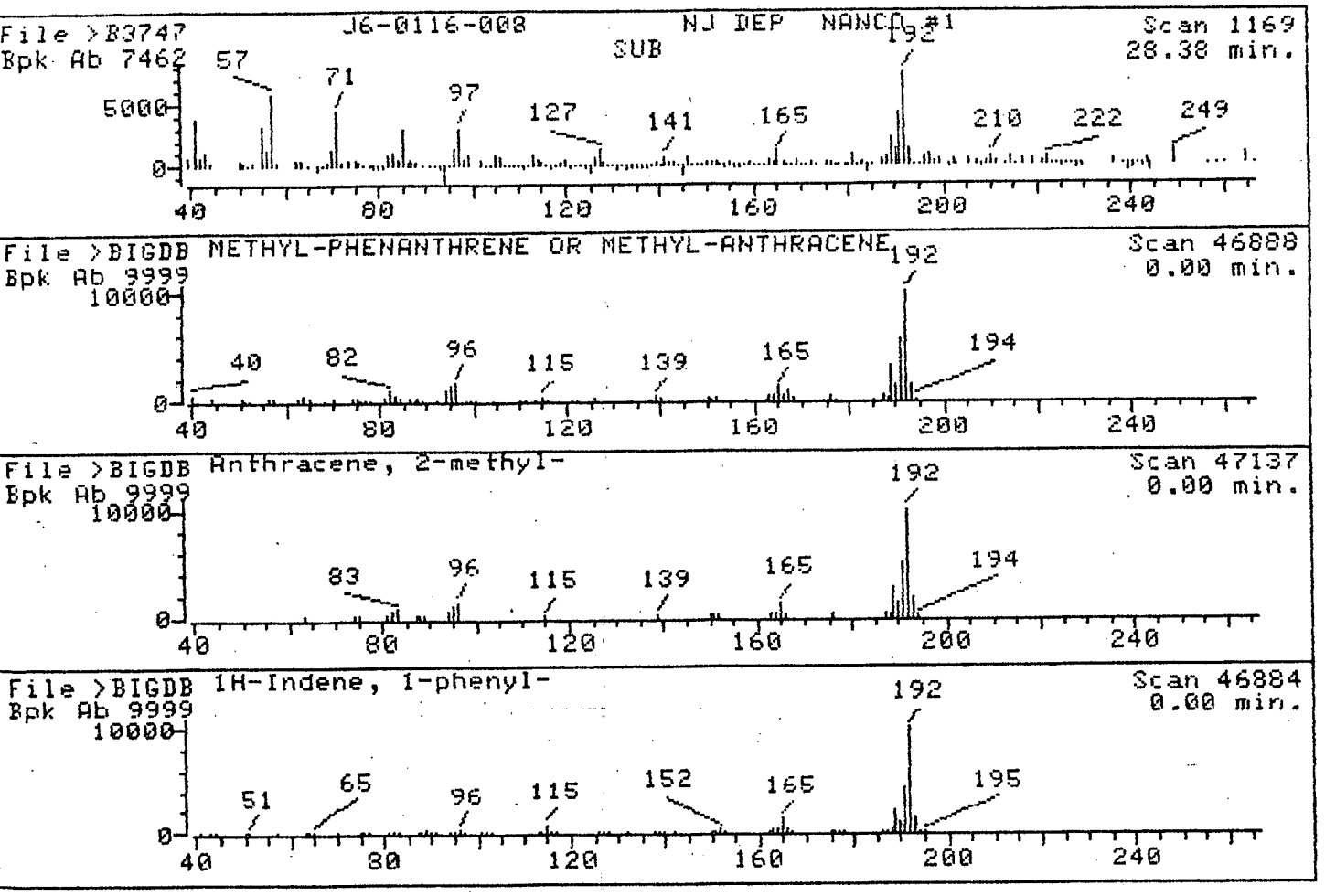
000303

1. Nonadecane
2. Octadecane
3. Eicosane
4. Heptadecane
5. Heneicosane

268 C19H40
254 C18H38
282 C20H42
240 C17H36
296 C21H44

Sample file: >B3747 Spectrum #: 1161
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	91*	629925	12414	"BIGDB	93	35	1	0	57	21	53	92
2.	89	593453	12800	"BIGDB	108	17	1	0	85	1	66	66
3.	89	112958	12426	"BIGDB	109	19	1	0	81	1	66	67
4.	89	629787	12796	"BIGDB	96	15	1	0	100	2	66	63
5.	89	629947	12449	"BIGDB	103	24	1	0	77	1	66	63

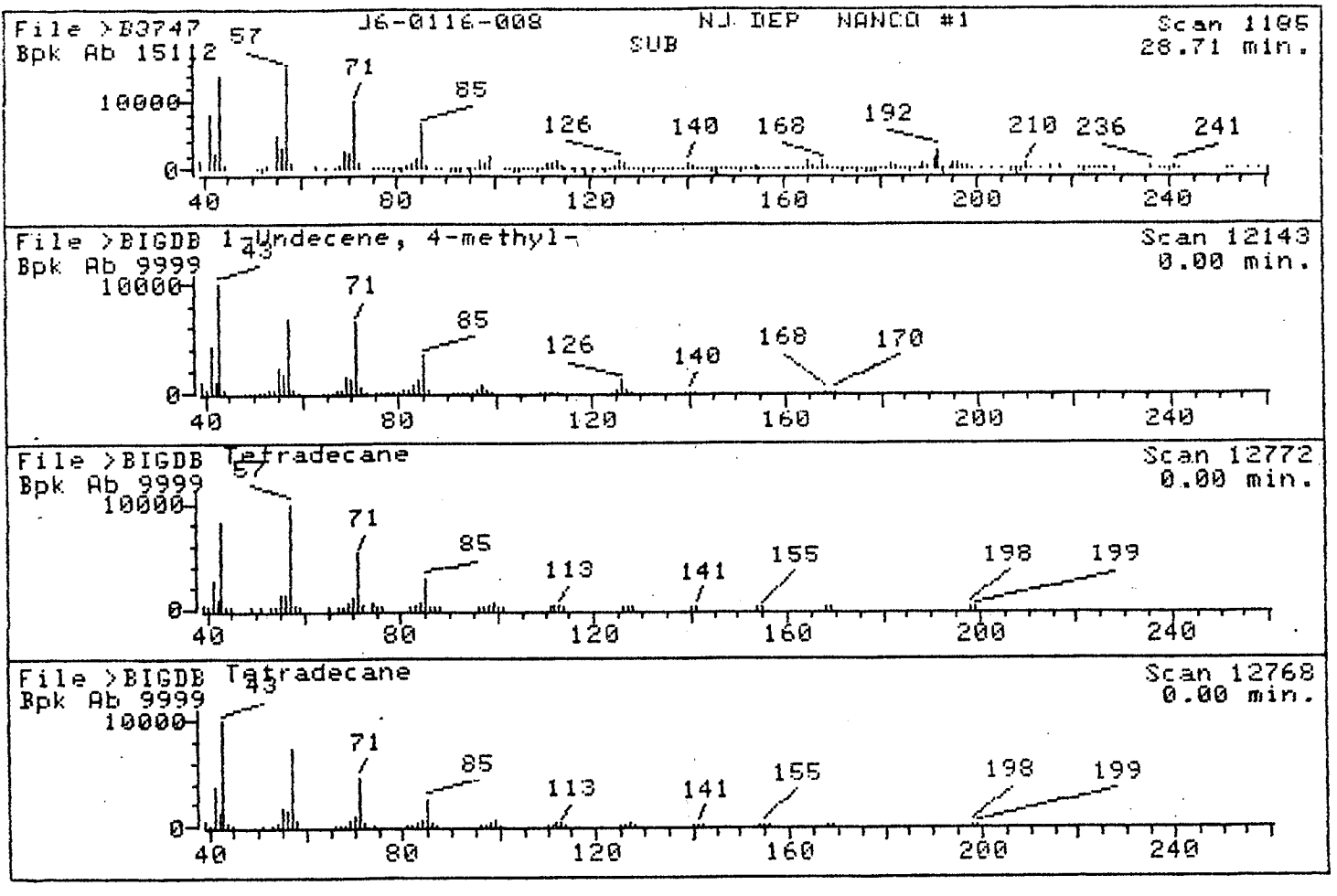


000304

1.	METHYL-PHENANTHRENE OR METHYL-ANTHRACENE	192 C15H12
2.	Anthracene, 2-methyl-	192 C15H12
3.	1H-Indene, 1-phenyl-	192 C15H12
4.	Phenanthrene, 2-methyl-	192 C15H12
5.	Phenanthrene, 4-methyl-	192 C15H12

Sample file: >B3747 Spectrum #: 1169
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	57*	0	46888	"BIGDB	89	28	2	0	100	46	14	67
2.	40*	613127	47137	"BIGDB	62	54	2	0	91	50	12	40
3.	38*	1961962	46884	"BIGDB	62	45	1	0	100	53	11	60
4.	35*	2531842	46880	"BIGDB	56	59	2	0	100	50	11	33
5.	32*	832644	46878	"BIGDB	83	33	3	0	86	51	9	49

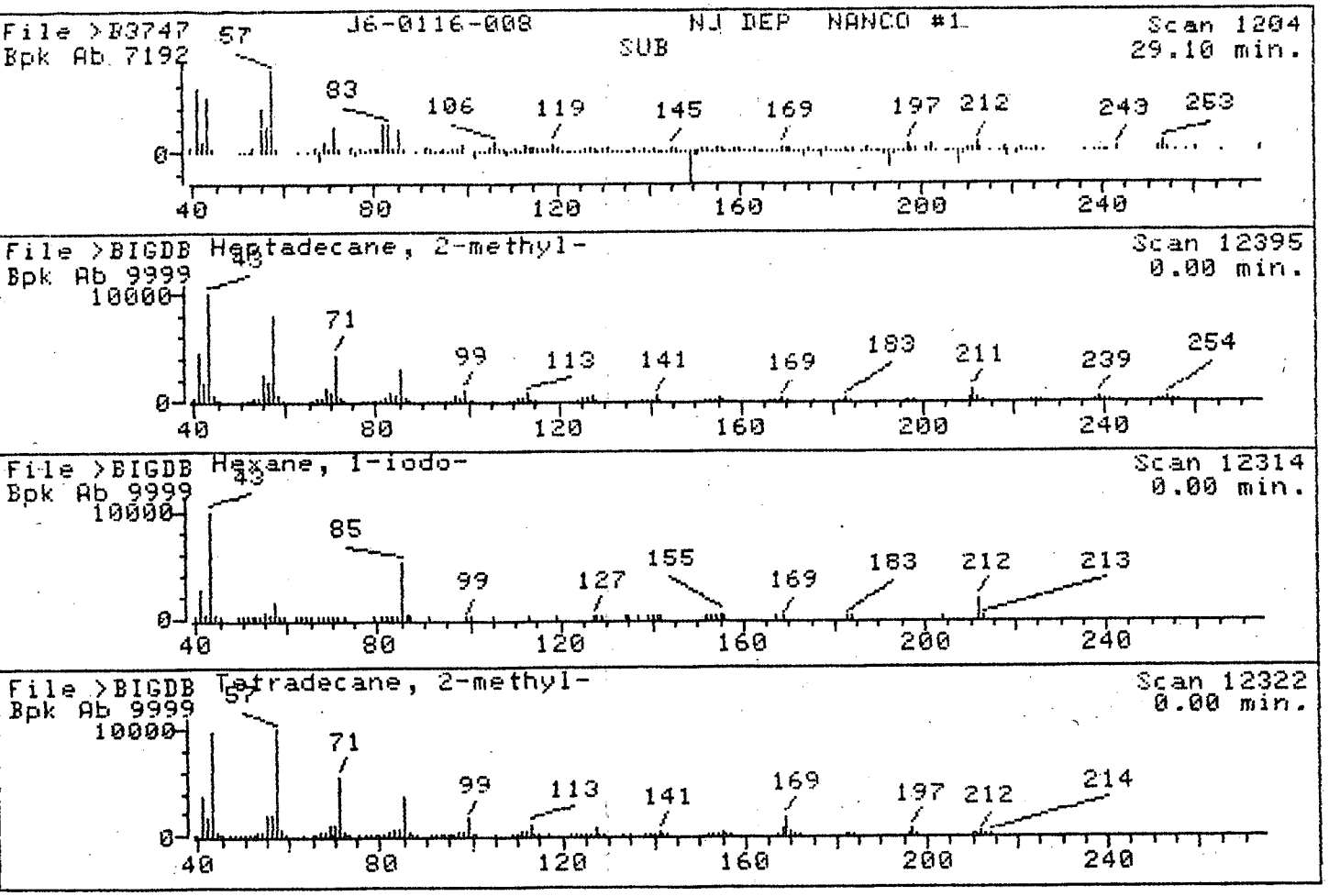


000305

1.	1-Undecene, 4-methyl-	168 C12H24
2.	Tetradecane	198 C14H30
3.	Tetradecane	198 C14H30
4.	Heneicosane	296 C21H44
5.	Hexadecane	226 C16H34

Sample file: >B3747 Spectrum #: 1185
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	87*	74630390	12143	"BIGDB	73	26	0	0	82	37	47	92
2.	83*	629594	12772	"BIGDB	73	35	1	0	100	14	51	72
3.	83*	629594	12768	"BIGDB	72	36	1	0	130	14	51	71
4.	79	629947	12449	"BIGDB	113	14	1	0	92	14	43	69
5.	76	544763	12781	"BIGDB	97	22	1	0	92	13	40	57

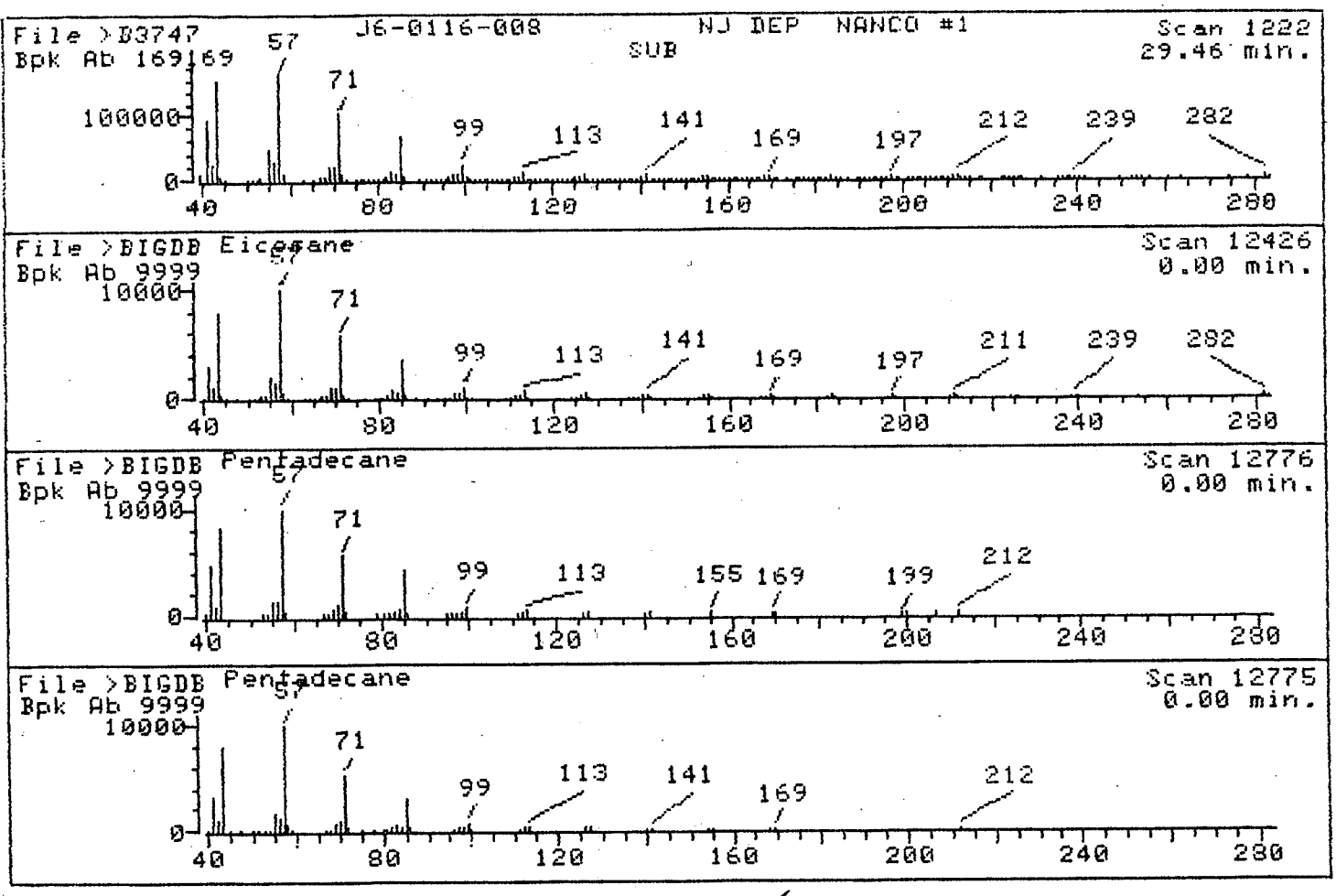


000306

1.	Heptadecane, 2-methyl-	254 C18H38
2.	Hexane, 1-iodo-	212 C6H13I
3.	Tetradecane, 2-methyl-	212 C15H32
4.	Pentadecane	212 C15H32
5.	Octadecane, 2-methyl-	268 C19H40

Sample file: >B3747 Spectrum #: 1204
Search speed: 1 Tilting option: N No. of ion ranges searched: 53

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	13*	1560890	12395	"BIGDB	60	69	2	0	67	63	3	37
2.	13*	638459	12314	"BIGDB	35	46	0	0	47	63	3	36
3.	13*	1560958	12322	"BIGDB	54	70	2	0	53	63	3	31
4.	12*	629629	12778	"BIGDB	50	63	2	0	67	63	2	23
5.	11	1560889	12412	"BIGDB	60	76	2	0	50	63	2	12

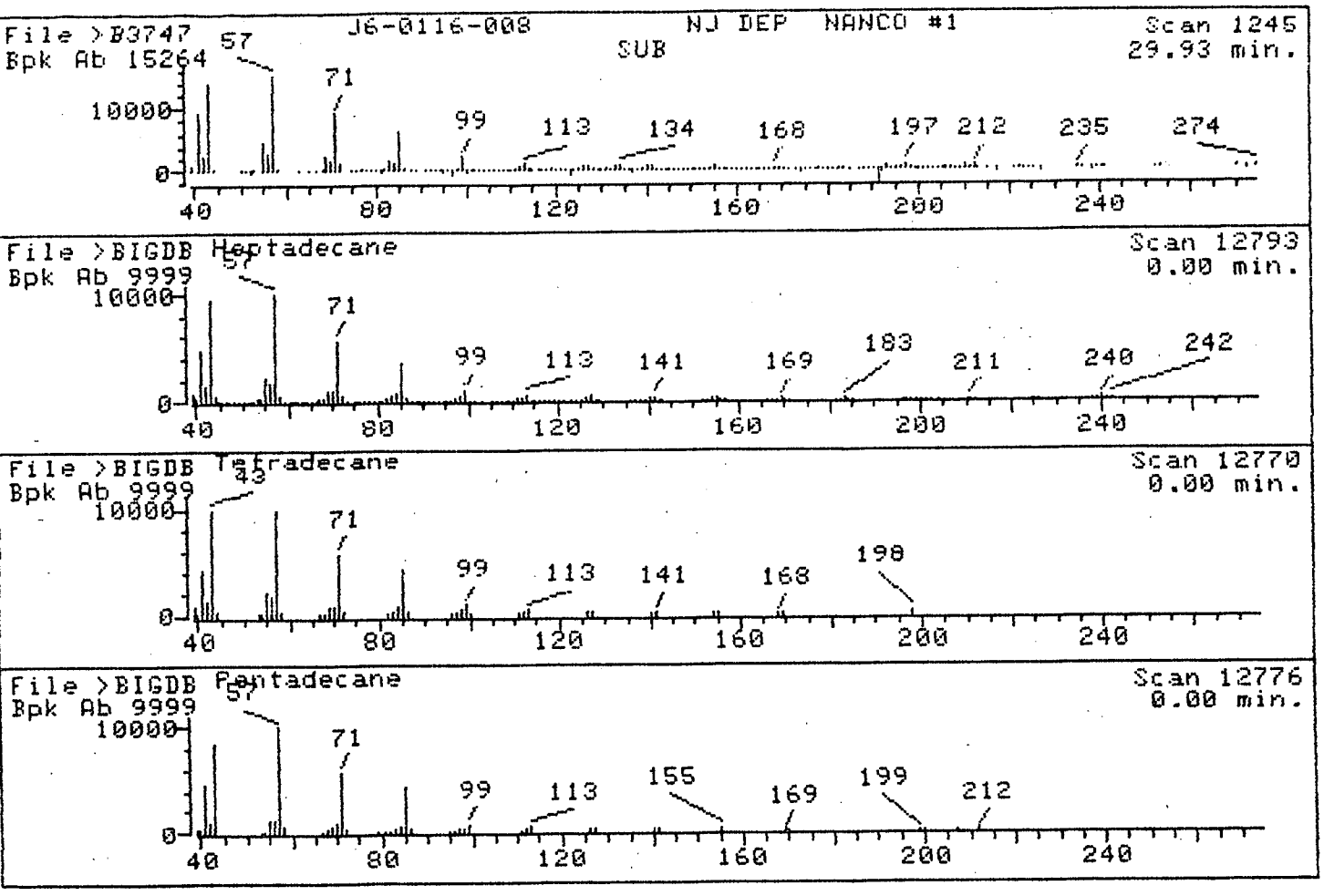


000307

1. Eicosane 282 C20H42
2. Pentadecane 212 C15H32
3. Pentadecane 212 C15H32
4. Pentadecane 212 C15H32
5. Eicosane 282 C20H42

Sample file: >B3747 Spectrum #: 1222
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	99*	112958	12426	"BIGDB	120	8	0	0	91	3	72	99
2.	96*	629629	12776	"BIGDB	103	6	1	0	90	3	72	96
3.	96*	629629	12775	"BIGDB	82	24	0	0	100	5	72	94
4.	95*	629629	12778	"BIGDB	90	23	0	0	74	19	60	96
5.	90*	112958	12815	"BIGDB	98	41	1	0	53	34	50	93

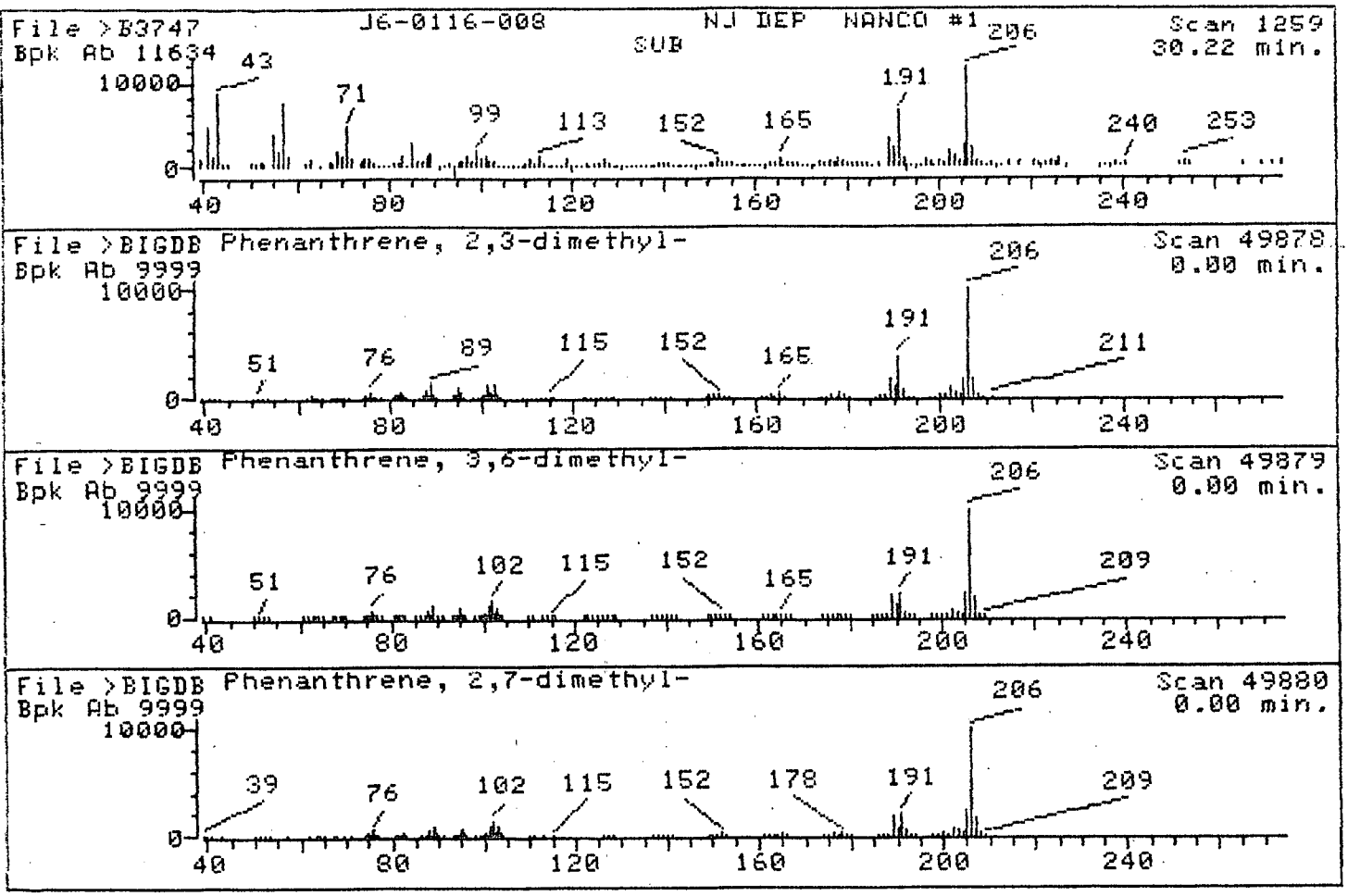


000308

1. Heptadecane 240 C17H36
2. Tetradecane 198 C14H30
3. Pentadecane 212 C15H32
4. Pentadecane 212 C15H32
5. Pentadecane 212 C15H32

Sample file: >B3747 Spectrum #: 1245
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	94*	629787	12793	"BIGDB	86	29	0	0	78	11	64	95
2.	87*	629594	12770	"BIGDB	89	29	1	0	79	12	55	89
3.	86*	629629	12776	"BIGDB	78	31	1	0	96	10	59	76
4.	86*	629629	12778	"BIGDB	71	42	1	0	100	10	59	71
5.	83*	629629	12323	"BIGDB	80	32	1	0	91	12	51	77

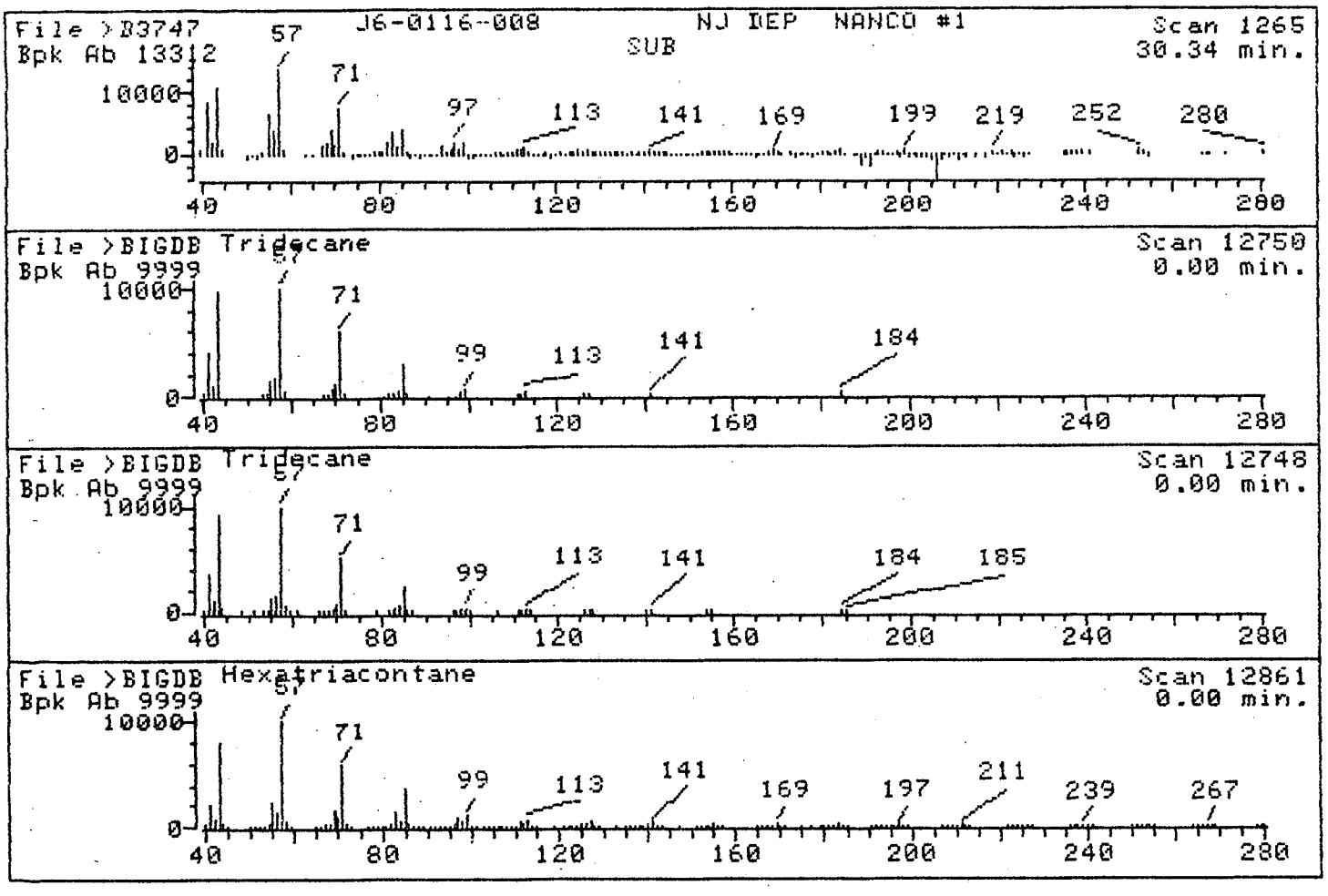


000309

1. Phenanthrene, 2,3-dimethyl- 206 C16H14
2. Phenanthrene, 3,6-dimethyl- 206 C16H14
3. Phenanthrene, 2,7-dimethyl- 206 C16H14
4. INDENE, 2-METHYL-3-PHENYL- 206 C16H14
5. Phenanthrene, 2,7-dimethyl- 206 C16H14

Sample file: >B3747 Spectrum #: 1259
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	52*	3674655	49878	"BIGDB	73	57	2	0	87	45	17	55
2.	52*	1576676	49879	"BIGDB	73	58	2	0	93	45	17	55
3.	47*	1576698	49880	"BIGDB	66	61	2	0	88	45	16	45
4.	36*	0	49897	"BIGDB	52	85	2	0	72	41	12	27
5.	35*	1576698	50052	"BIGDB	57	65	2	0	87	50	11	34

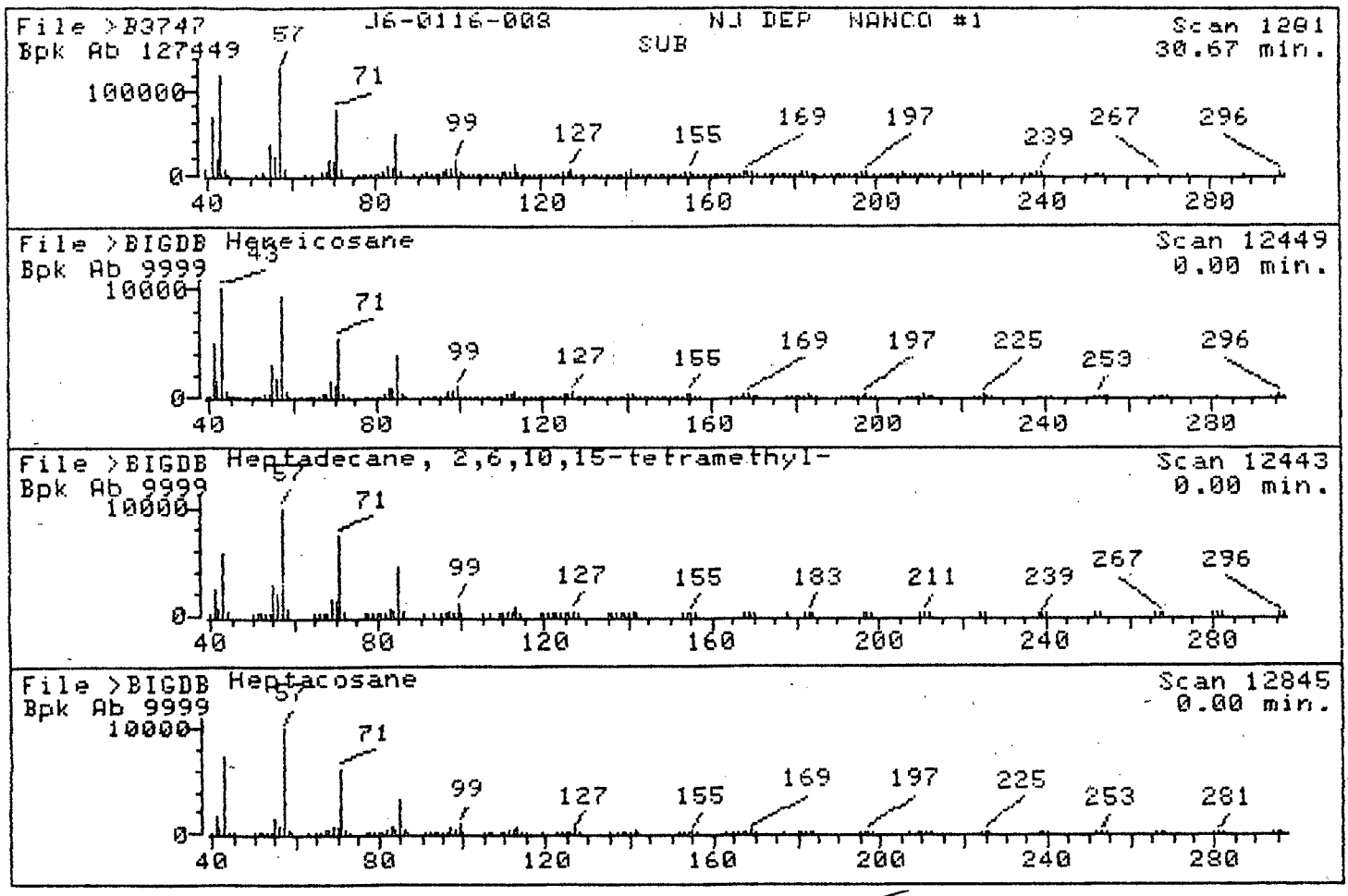


000310

1.	Tridecane	184 C13H28
2.	Tridecane	184 C13H28
3.	Hexatriacontane	506 C36H74
4.	Hexatriacontane	506 C36H74
5.	Pentatriacontane	492 C35H72

Sample file: >B3747 Spectrum #: 1265
Search speed: 1 Tilting option: N No. of ion ranges searched: 48

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	75*	629505	12750	"BIGDB	60	47	0	0	76	27	37	73
2.	71*	629505	12748	"BIGDB	53	53	0	0	88	27	29	65
3.	70	630068	12861	"BIGDB	92	69	1	0	75	18	32	50
4.	66	630068	12862	"BIGDB	105	48	2	0	68	18	31	40
5.	63	630079	12543	"BIGDB	97	54	2	0	67	18	30	31



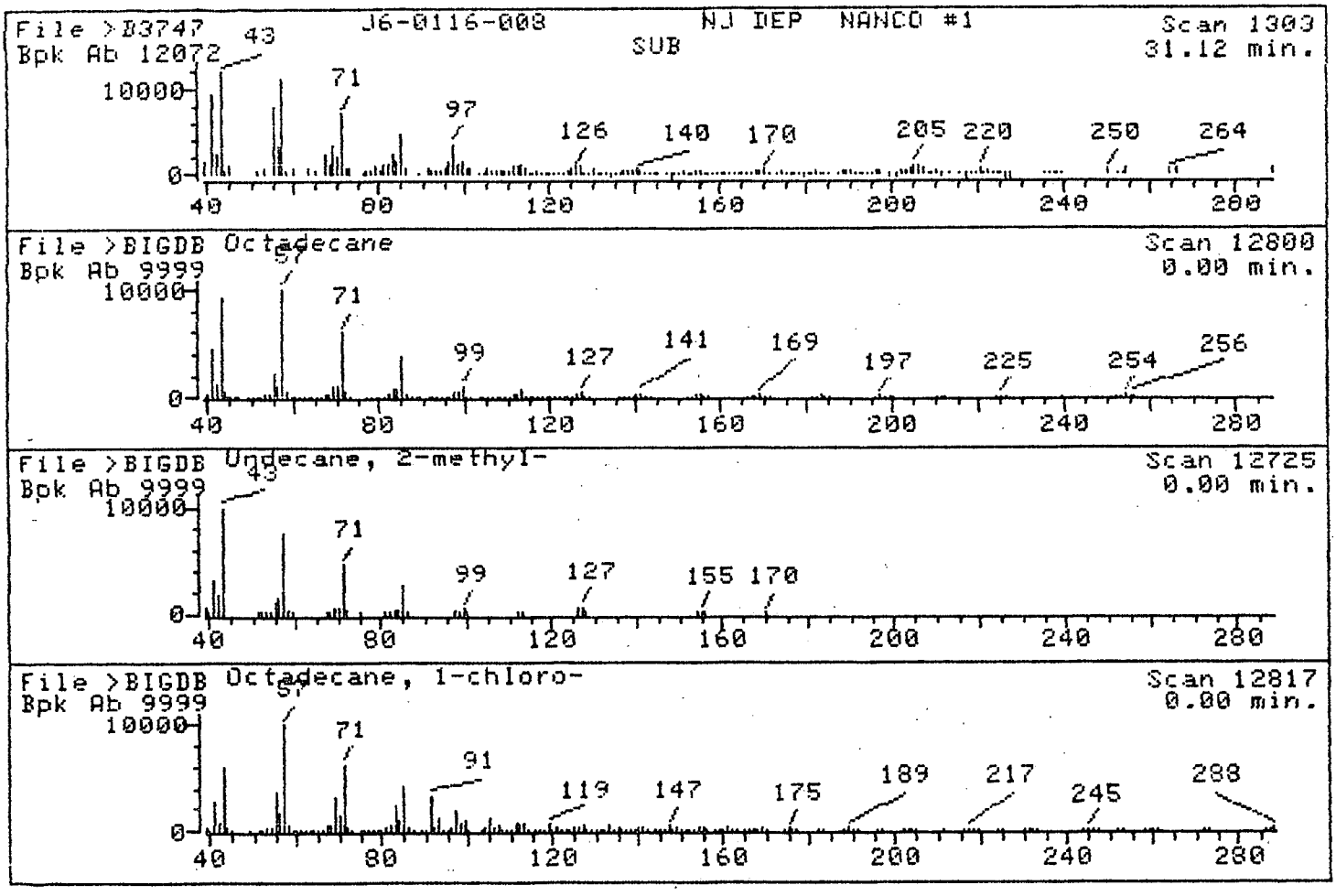
Unk Hyd 16

000311

1. Heneicosane	296	C21H44
2. Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44
3. Heptacosane	380	C27H56
4. Pentacosane	352	C25H52
5. Octadecane	254	C18H38

Sample file: >B3747 Spectrum #: 1281
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	96*	629947	12449	"BIGDB	108	19	1	0	85	0	72	96
2.	92*	54833486	12443	"BIGDB	98	35	1	0	65	23	53	93
3.	89	593497	12845	"BIGDB	118	9	1	0	90	1	66	76
4.	89	629992	12483	"BIGDB	125	19	1	0	72	1	66	77
5.	89	593453	12800	"BIGDB	113	12	1	0	86	1	66	71



000312

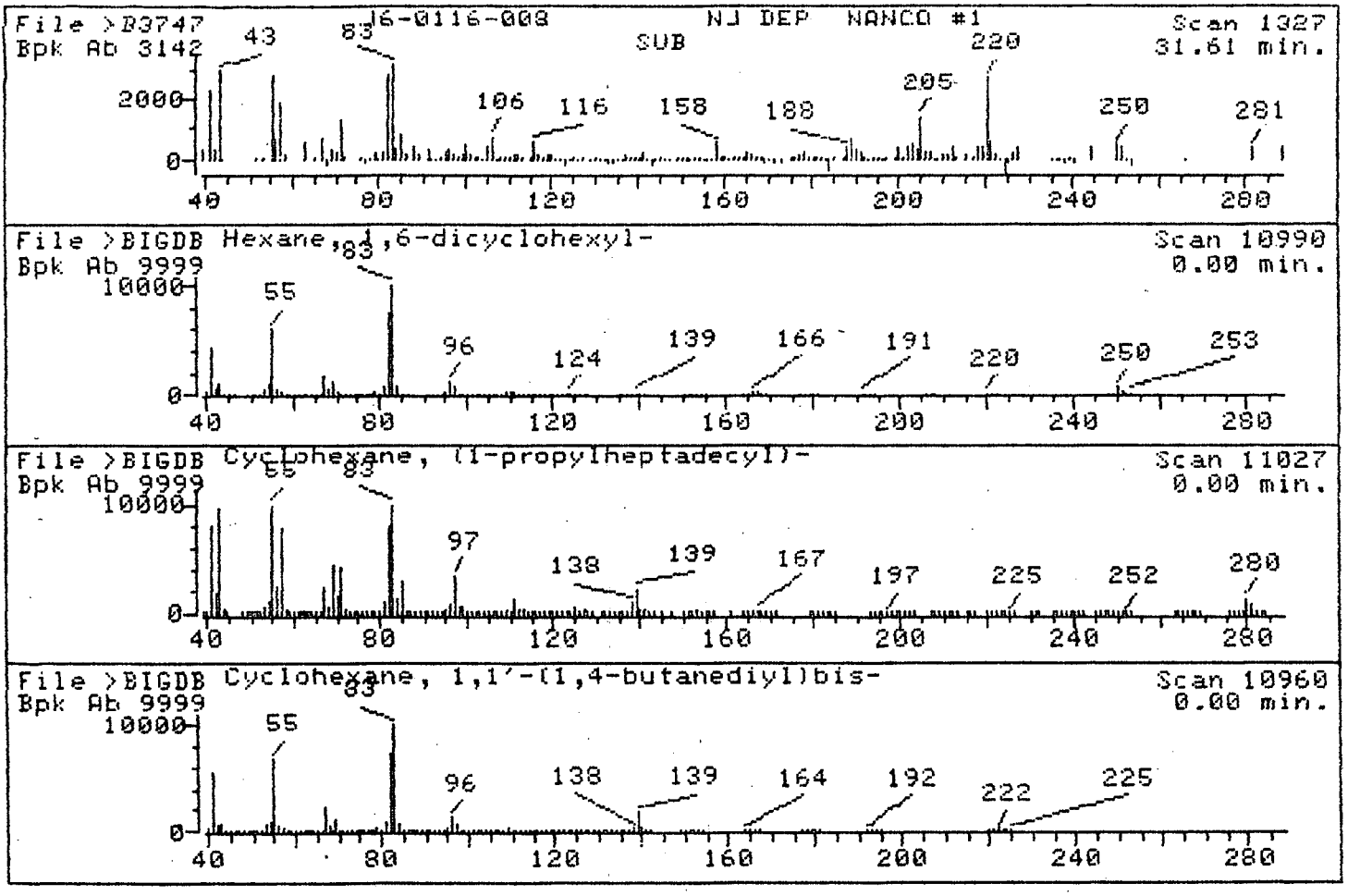
UNL

Hydr

1. Octadecane — 254 C18H38
2. Undecane, 2-methyl- — 170 C12H26
3. Octadecane, 1-chloro- — 288 C18H37Cl
4. Dodecane — 170 C12H26
5. Nonane, 3,7-dimethyl- — 156 C11H24

Sample file: >B3747 Spectrum #: 1303
Search speed: 1 Tilting option: N No. of ion ranges searched: 57

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	67*	593453	12800	"BIGDB	77	48	1	0	72	43	24	74
2.	61*	7045718	12725	"BIGDB	54	40	0	0	100	45	18	66
3.	59*	3386332	12817	"BIGDB	70	70	2	0	85	36	21	50
4.	56*	112403	12727	"BIGDB	54	43	0	0	99	47	14	66
5.	47*	17302328	12095	"BIGDB	38	48	0	0	62	45	16	44

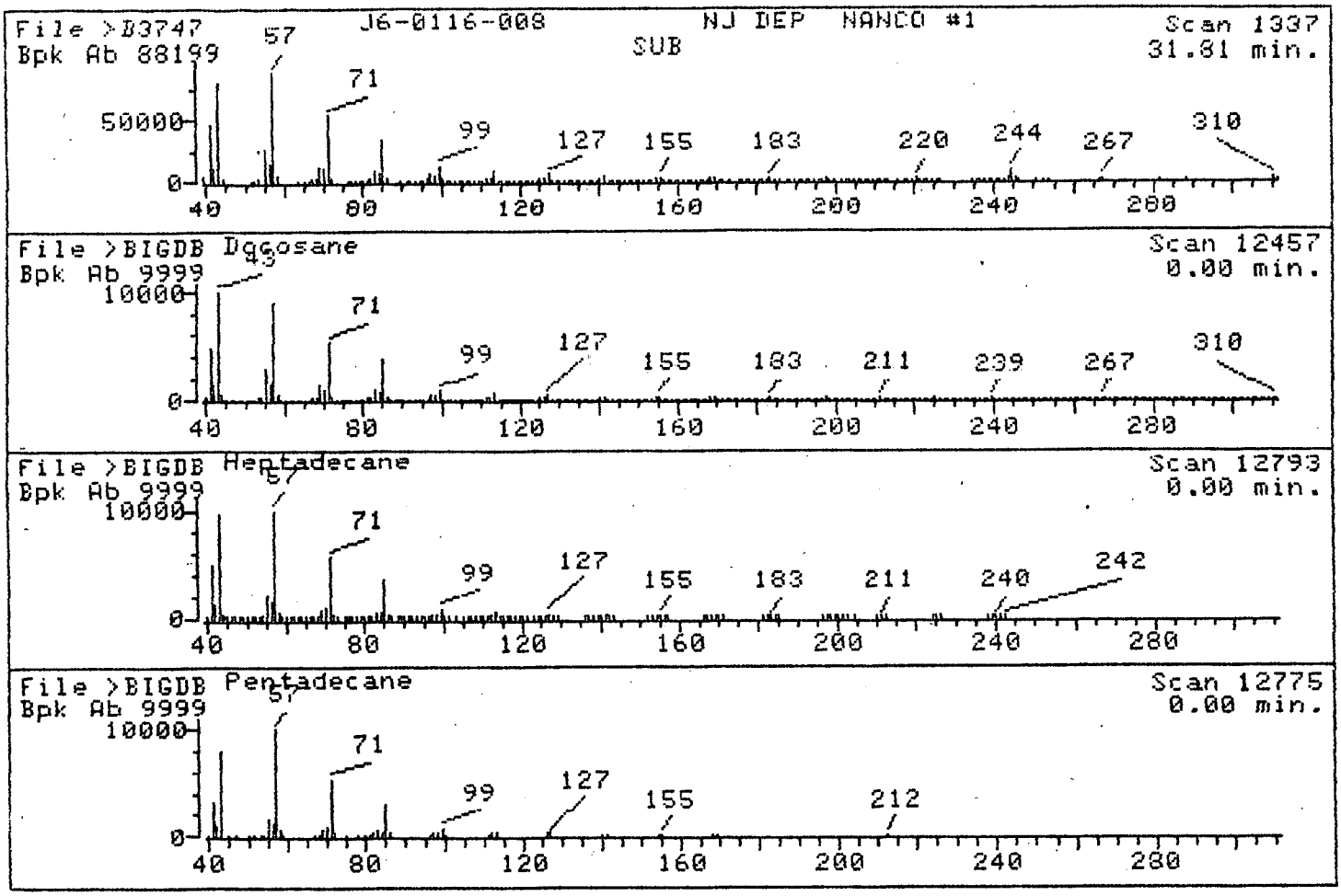


000313

1. Hexane, 1,6-dicyclohexyl-	250	C18H34
2. Cyclohexane, (1-propylheptadecyl)-	364	C26H52
3. Cyclohexane, 1,1'-(1,4-butanediyl)bis-	222	C16H30
4. Heptanenitrile	111	C7H13N
5. 1-Azabicyclo[3.1.0]hexane	83	C5H9N

Sample file: >B3747 Spectrum #: 1327
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	25*	1610237	10990	"BIGDB	42	77	2	0	81	50	7	14
2.	25	4443587	11027	"BIGDB	88	83	3	0	76	50	7	17
3.	20*	6165442	10960	"BIGDB	54	68	3	0	100	52	5	17
4.	20*	629083	10774	"BIGDB	40	62	3	0	88	52	5	13
5.	20*	285767	10749	"BIGDB	27	52	3	0	174	52	5	13



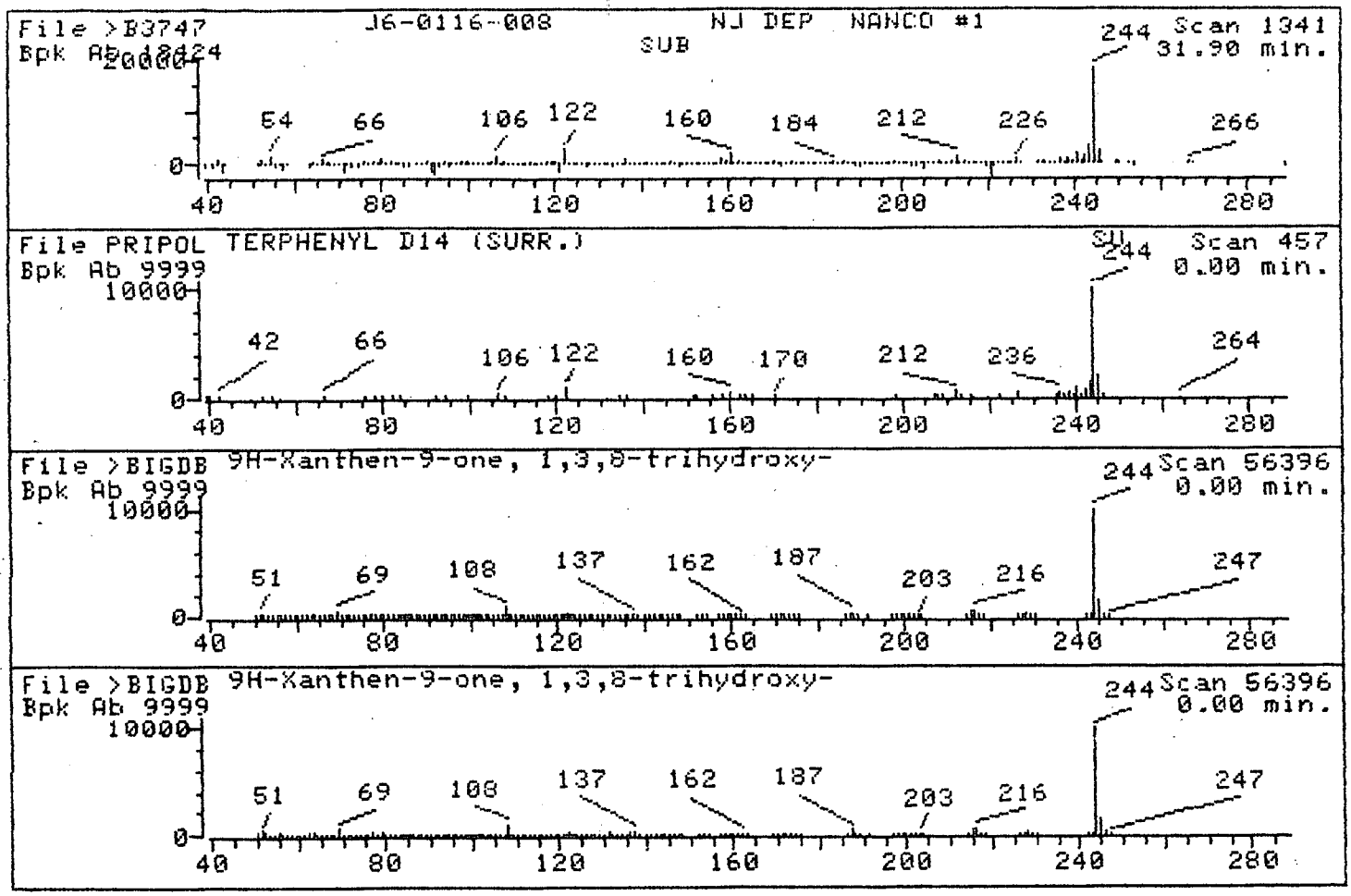
000314

Hydr

1.	Docosane	310	C22H46
2.	Heptadecane	240	C17H36
3.	Pentadecane	212	C15H32
4.	Pentacosane	352	C25H52
5.	Heptadecane	240	C17H36

Sample file: >B3747 Spectrum #: 1337
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	99*	629970	12457	"BIGDB	123	9	1	0	87	10	68	99
2.	99*	629787	12793	"BIGDB	111	4	0	0	83	9	68	99
3.	95*	629629	12775	"BIGDB	81	25	0	0	100	10	68	94
4.	94	629992	12483	"BIGDB	141	3	0	0	83	11	64	94
5.	94*	629787	12796	"BIGDB	80	31	0	0	100	12	64	94

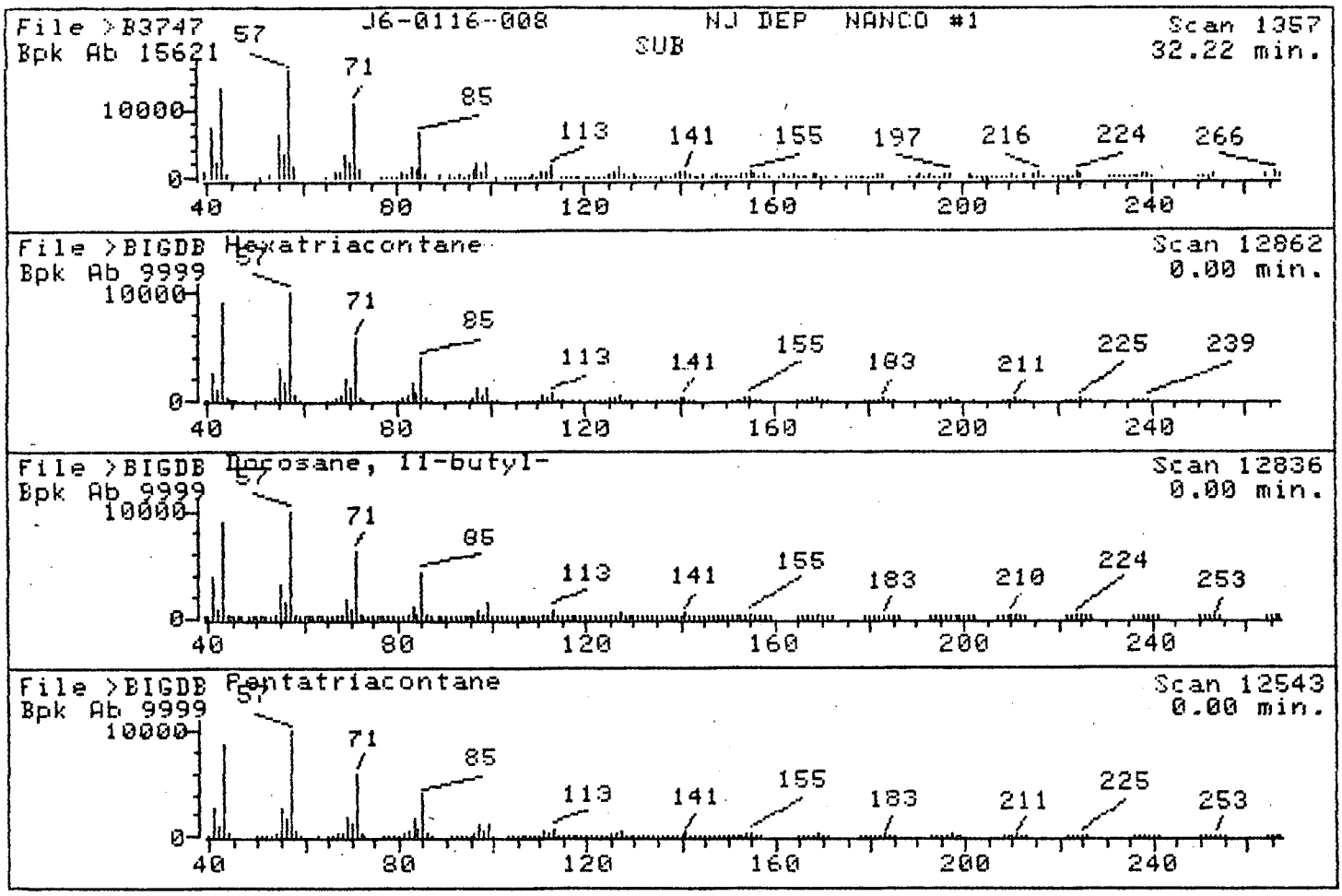


000315

1. TERPHENYL D14 (SURR.) SU 244
RROGATE COMPOUND BNA
SURROGATE
2. 9H-Xanthen-9-one, 1,3,8-trihydroxy- 244 C13H8O5

Sample file: >B3747 Spectrum #: 1341
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	67*	457	403	PRIPOL	72	65	1	0	57	39	28	71
2.	28*	6052933	56396	"BIGDB	29	88	2	0	99	37	10	14

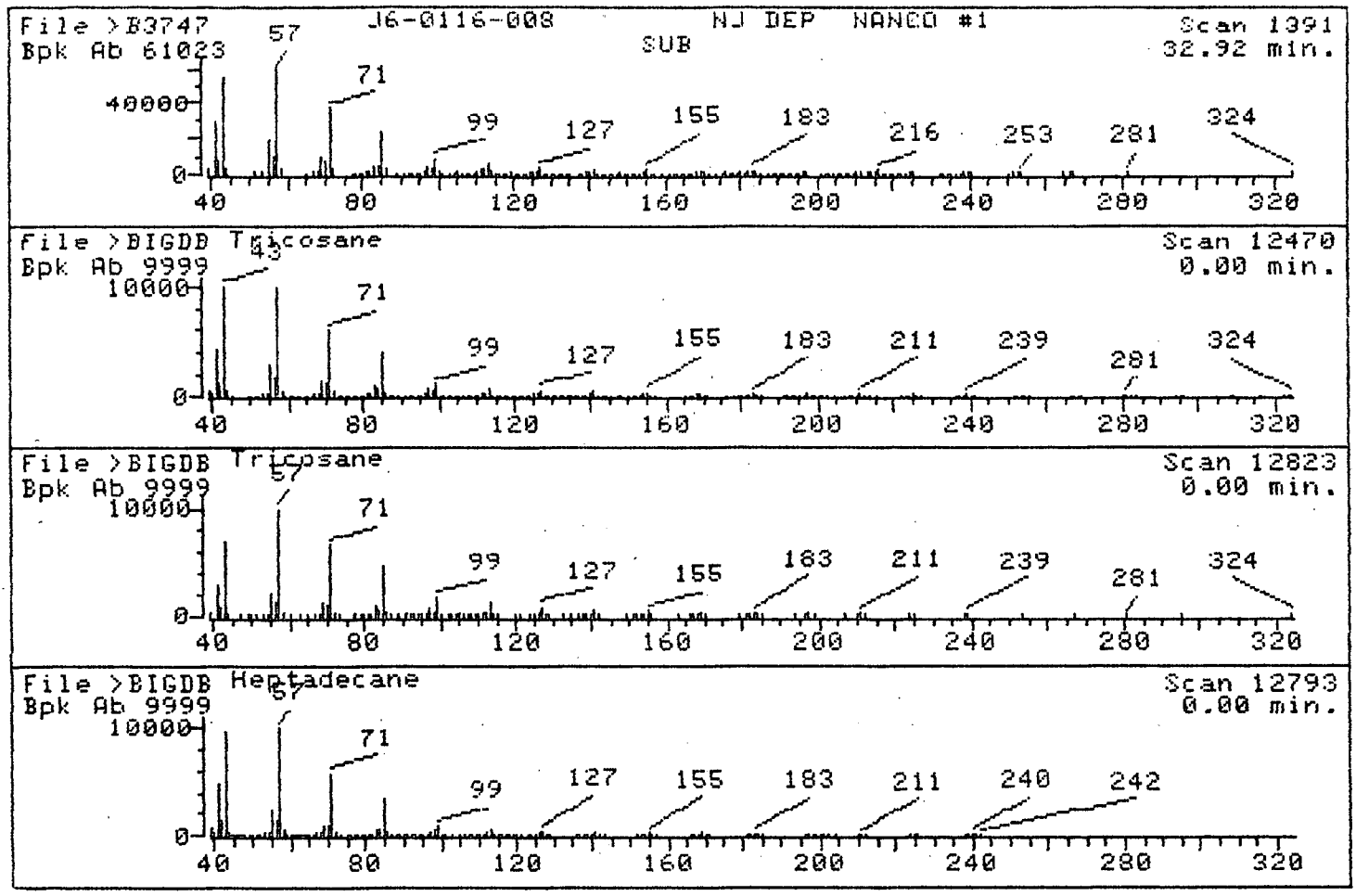


000316

1. Hexatriacontane	506	C36H74
2. Docosane, 11-butyl-	366	C26H54
3. Pentatriacontane	492	C35H72
4. Dotriacontane	450	C32H66
5. Docosane, 9-butyl-	366	C26H54

Sample file: >B3747 Spectrum #: 1357
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89	630068	12862	"BIGDB	121	32	2	0	92	4	66	60
2.	87	13475768	12836	"BIGDB	108	43	2	0	94	4	63	44
3.	87	630079	12543	"BIGDB	107	44	2	0	95	4	63	44
4.	87	544854	12534	"BIGDB	110	47	2	0	90	4	63	49
5.	86	55282149	12837	"BIGDB	104	47	2	0	95	4	60	39

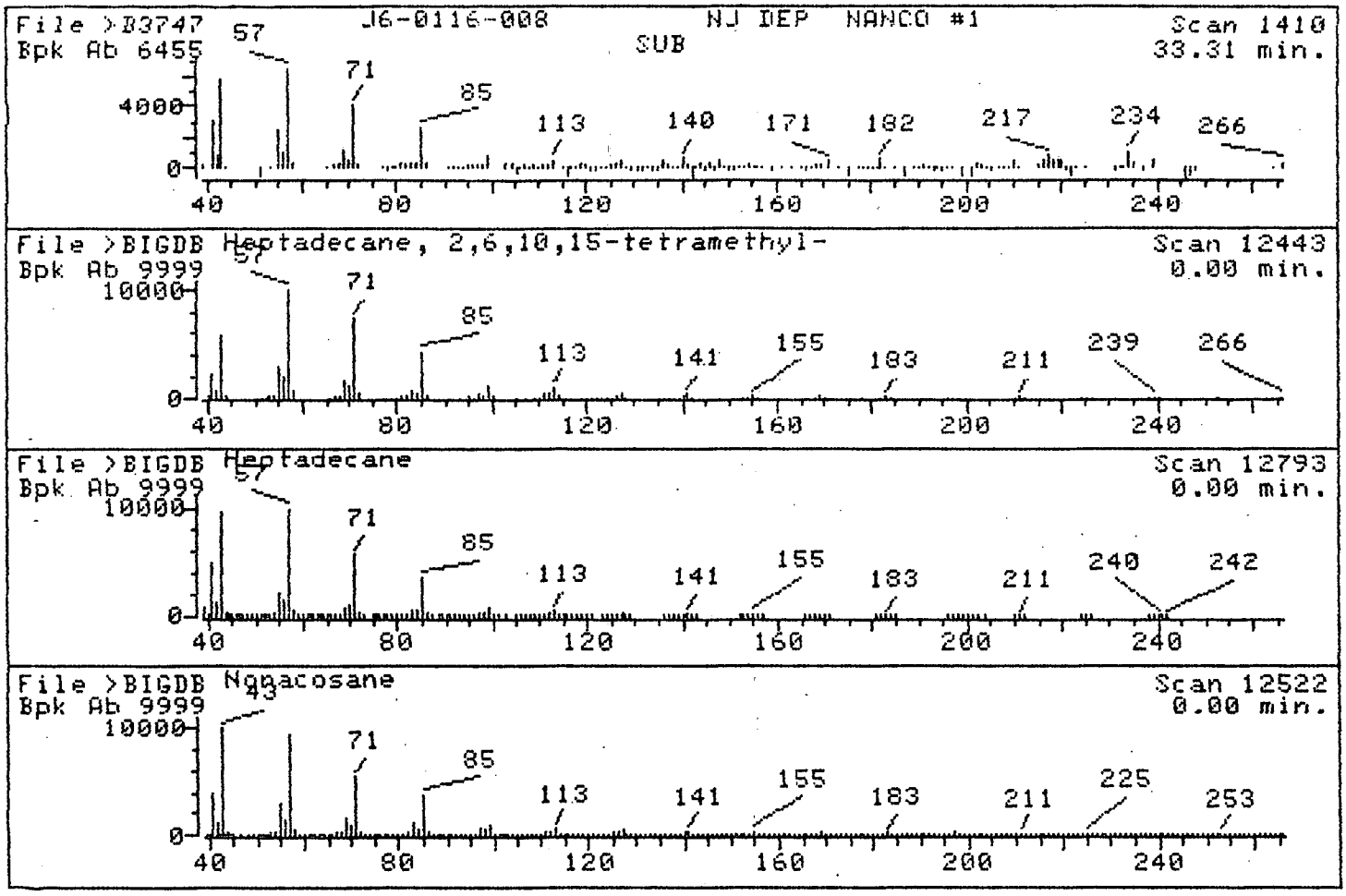


000317

1. Tricosane	324	C23H48
2. Tricosane	324	C23H48
3. Heptadecane	240	C17H36
4. Heptadecane	240	C17H36
5. Heptacosane	380	C27H56

Sample file: >B3747 Spectrum #: 1391
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	99*	638675	12470	"BIGDB	122	16	1	0	78	3	72	99
2.	97*	638675	12823	"BIGDB	118	27	0	0	57	23	53	99
3.	96*	629787	12793	"BIGDB	111	4	1	0	88	3	72	96
4.	96*	629787	12796	"BIGDB	91	20	0	0	100	8	68	96
5.	93	593497	12845	"BIGDB	123	4	1	0	97	5	68	80

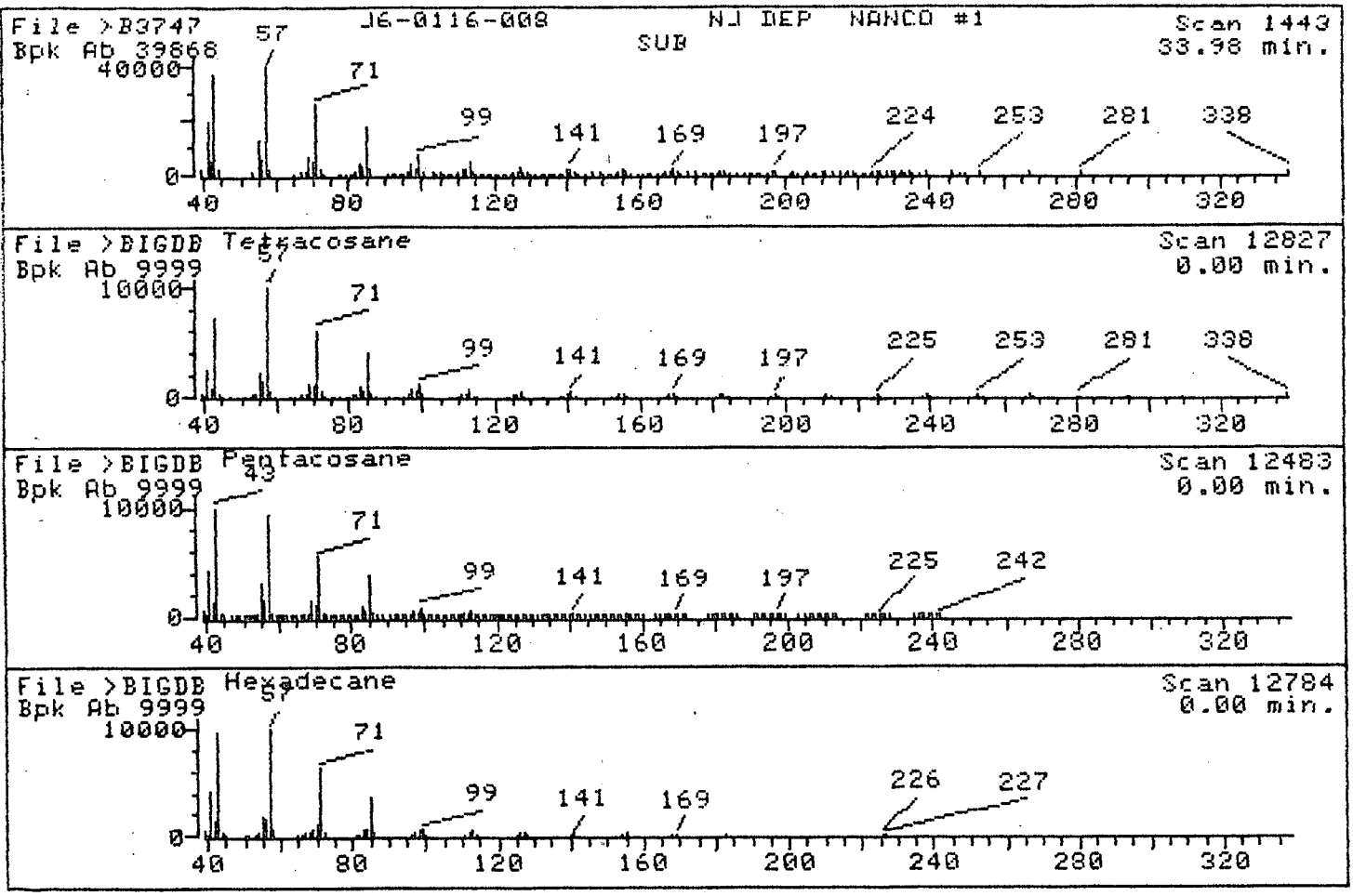


000318

1.	Heptadecane, 2,6,10,15-tetramethyl-	296 C21H44
2.	Heptadecane	240 C17H36
3.	Nonacosane	408 C29H60
4.	Hexatriacontane	506 C36H74
5.	Heptadecane	240 C17H36

Sample file: >B3747 Spectrum #: 1410
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	58	54833486	12443	"BIGDB	90	43	1	0	64	40	19	49
2.	46	629787	12793	"BIGDB	90	25	2	0	95	40	17	35
3.	41	630035	12522	"BIGDB	94	51	2	0	91	40	14	28
4.	41	630068	12862	"BIGDB	96	57	2	0	84	40	17	30
5.	41	629787	12796	"BIGDB	74	37	1	0	84	40	14	28

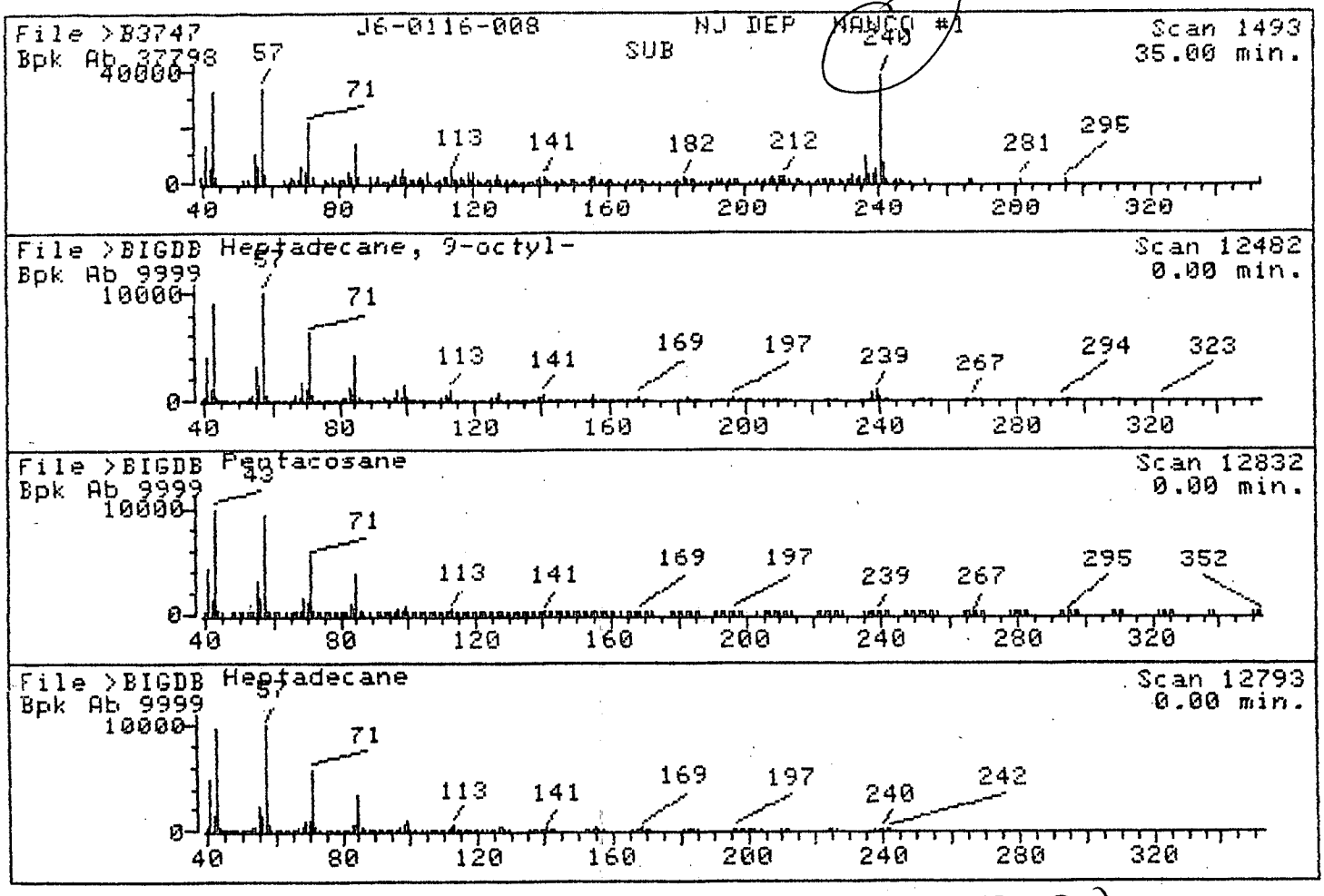


000319

1. Tetracosane	338	C24H50
2. Pentacosane	352	C25H52
3. Hexadecane	226	C16H34
4. Tetracosane	338	C24H50
5. Heptacosane	380	C27H56

Sample file: >B3747 Spectrum #: 1443
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	96*	646311	12827	"BIGDB	100	37	1	0	81	5	72	94
2.	94	629992	12483	"BIGDB	136	8	0	0	86	6	68	93
3.	92*	544763	12784	"BIGDB	74	45	0	0	84	12	64	92
4.	88	646311	12476	"BIGDB	117	25	2	0	79	3	65	56
5.	88	593497	12846	"BIGDB	118	35	2	0	69	5	65	57



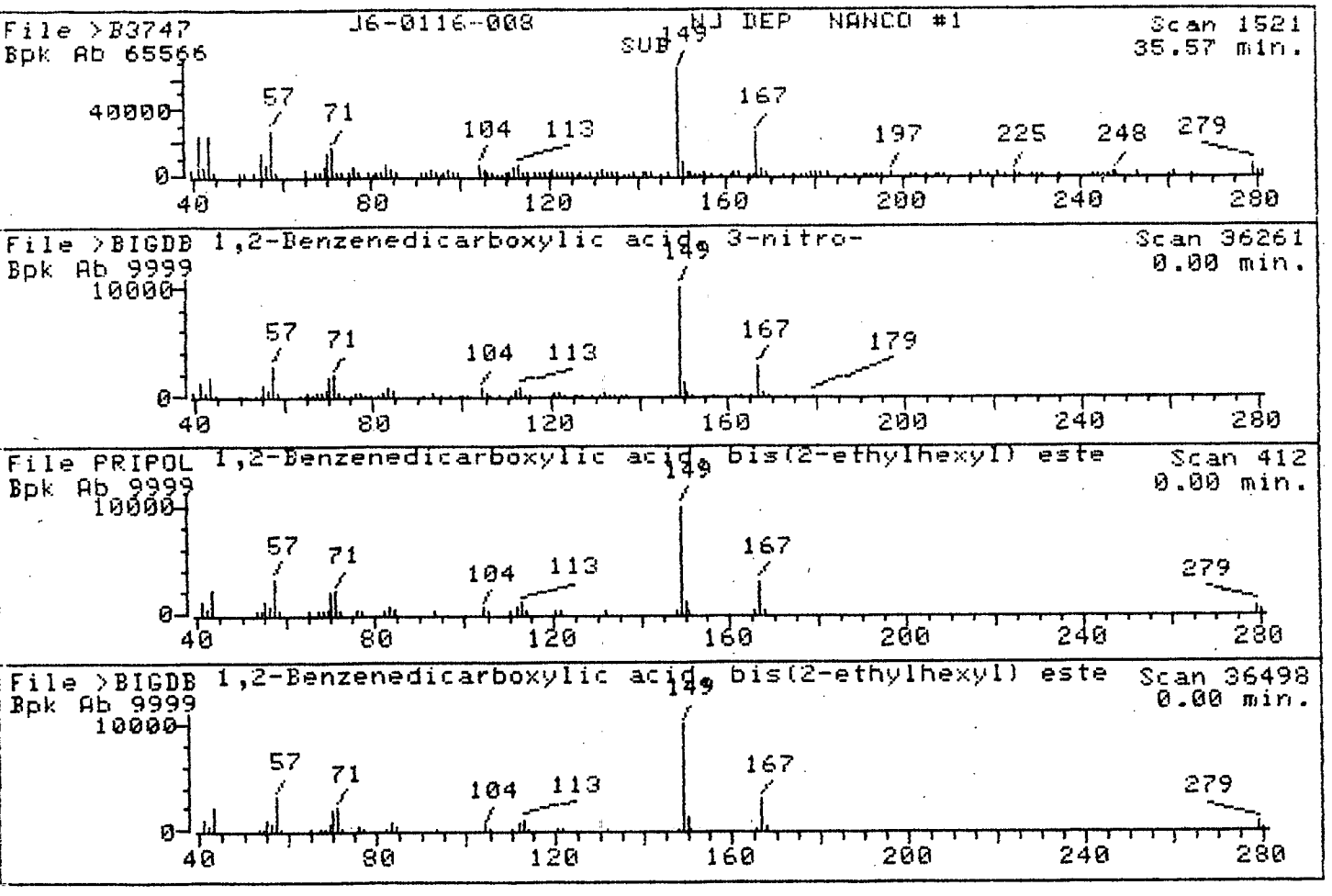
Chrysene d12 (ISTD)

000320

1. Heptadecane, 9-octyl- 352 C25H52
2. Pentacosane 352 C25H52
3. Heptadecane 240 C17H36
4. Heptadecane 240 C17H36
5. Pentadecane 212 C15H32

Sample file: >B3747 Spectrum #: 1493
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	54*	7225641	12482	"BIGDB	123	20	1	0	73	61	17	99
2.	44*	629992	12832	"BIGDB	122	18	1	0	82	68	11	99
3.	42*	629787	12793	"BIGDB	100	15	0	0	88	68	11	97
4.	42*	629787	12377	"BIGDB	96	26	0	0	89	68	11	97
5.	34*	629629	12323	"BIGDB	79	33	0	0	78	70	11	94

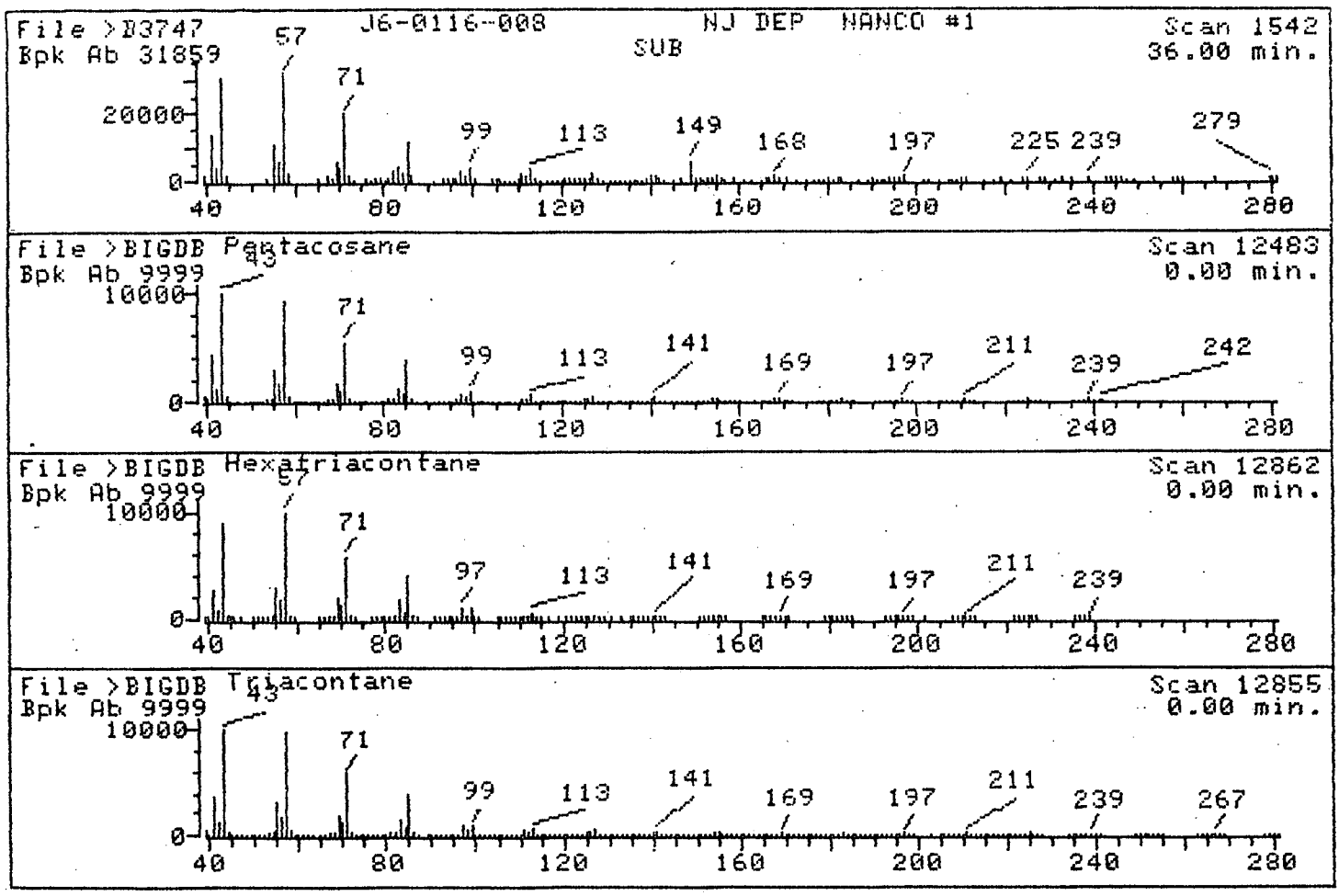


bis (2 eth hex) pth /16 000321

1. 1,2-Benzenedicarboxylic acid, 3-nitro- 211 C8H5NO6
2. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) este 390 C24H38O4
3. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) este 390 C24H38O4
4. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) este 390 C24H38O4
5. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) este 390 C24H38O4

Sample file: >B3747 Spectrum #: 1521
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89	603112	36261	"BIGDB	103	5	0	0	100	6	62	86
2.	89	412	247	PRIPOL	101	36	1	0	91	0	66	60
3.	89	117817	36498	"BIGDB	101	36	1	0	91	0	66	60
4.	86	117817	36390	"BIGDB	101	46	2	0	87	4	60	35
5.	86	408	243	PRIPOL	101	46	2	0	87	4	60	35

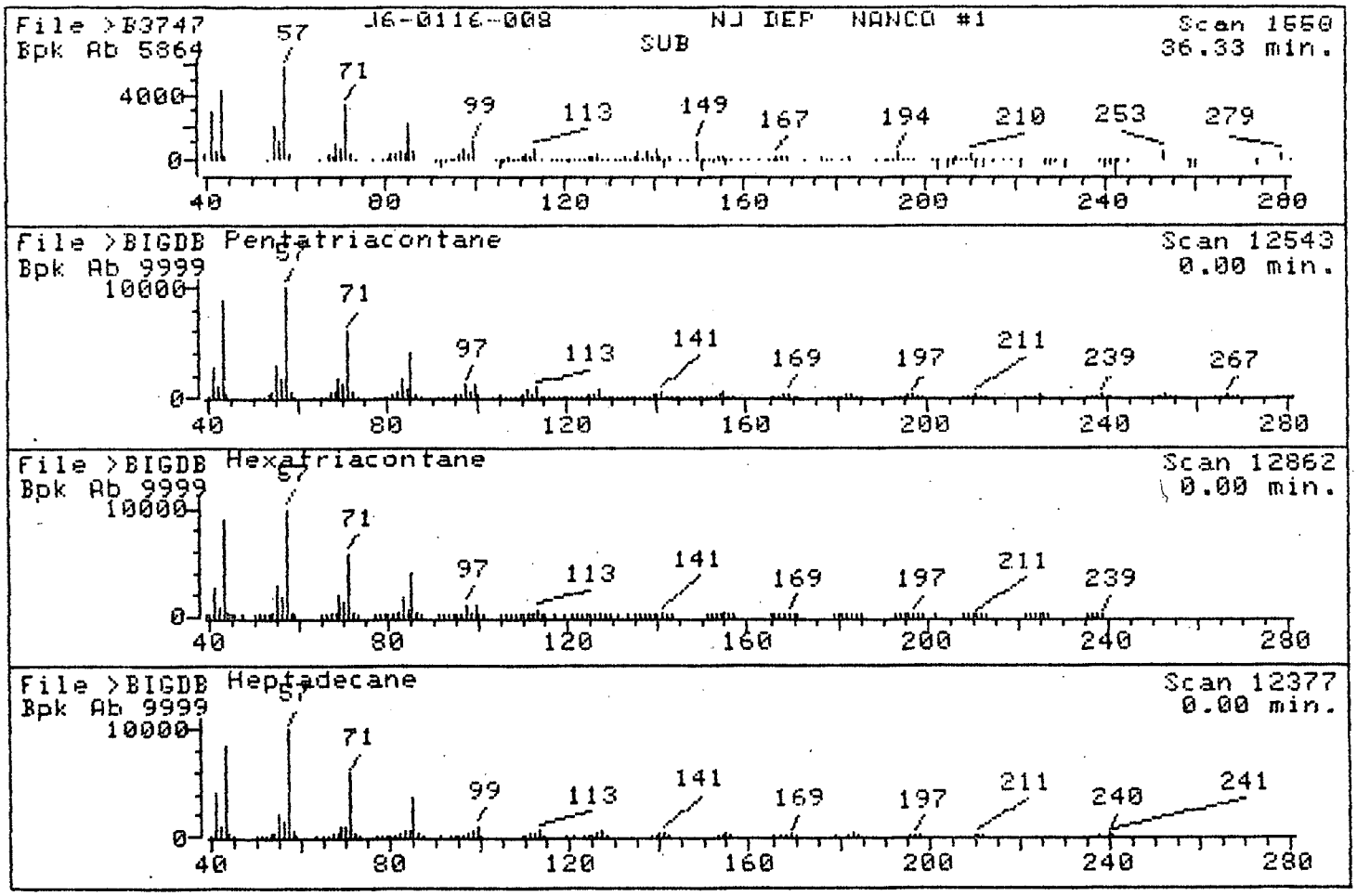


000322

1. Pentacosane	352	C25H52
2. Hexatriacontane	506	C36H74
3. Triacontane	422	C30H62
4. Octacosane	394	C28H58
5. Octacosane	394	C28H58

Sample file: >B3747 Spectrum #: 1542
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	93	629992	12483	"BIGDB	136	8	0	0	85	11	64	93
2.	83	630068	12862	"BIGDB	129	24	1	0	83	11	51	78
3.	83	638686	12855	"BIGDB	129	25	1	0	81	11	51	78
4.	83	630024	12848	"BIGDB	123	21	1	0	86	11	51	76
5.	83	630024	12516	"BIGDB	114	23	1	0	88	13	51	71

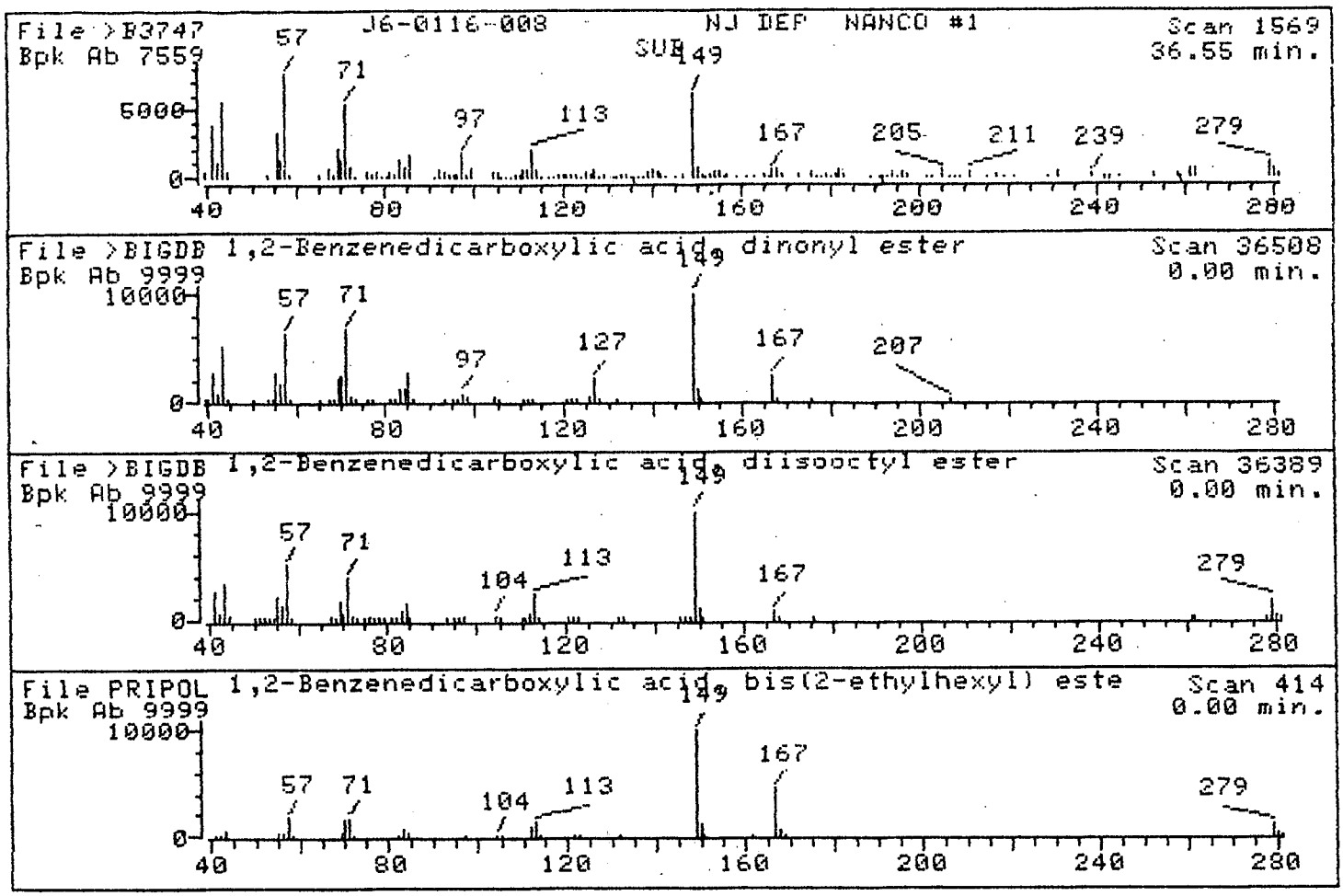


000323

1. Pentatriacontane	492	C35H72
2. Hexatriacontane	506	C36H74
3. Heptadecane	240	C17H36
4. Octacosane	394	C28H58
5. Eicosane, 10-methyl-	296	C21H44

Sample file: >B3747 Spectrum #: 1558
Search speed: 1 Tilting option: N No. of ion ranges searched: 49

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
* 1.	57	630079	12543	"BIGDB	106	45	2	0	76	33	22	42
2.	55	630068	12862	"BIGDB	104	49	2	0	82	31	20	39
3.	53	629787	12377	"BIGDB	88	34	1	0	88	38	19	44
4.	52	630024	12848	"BIGDB	102	42	2	0	93	33	20	36
5.	51	54833237	12445	"BIGDB	101	32	2	0	84	33	20	35

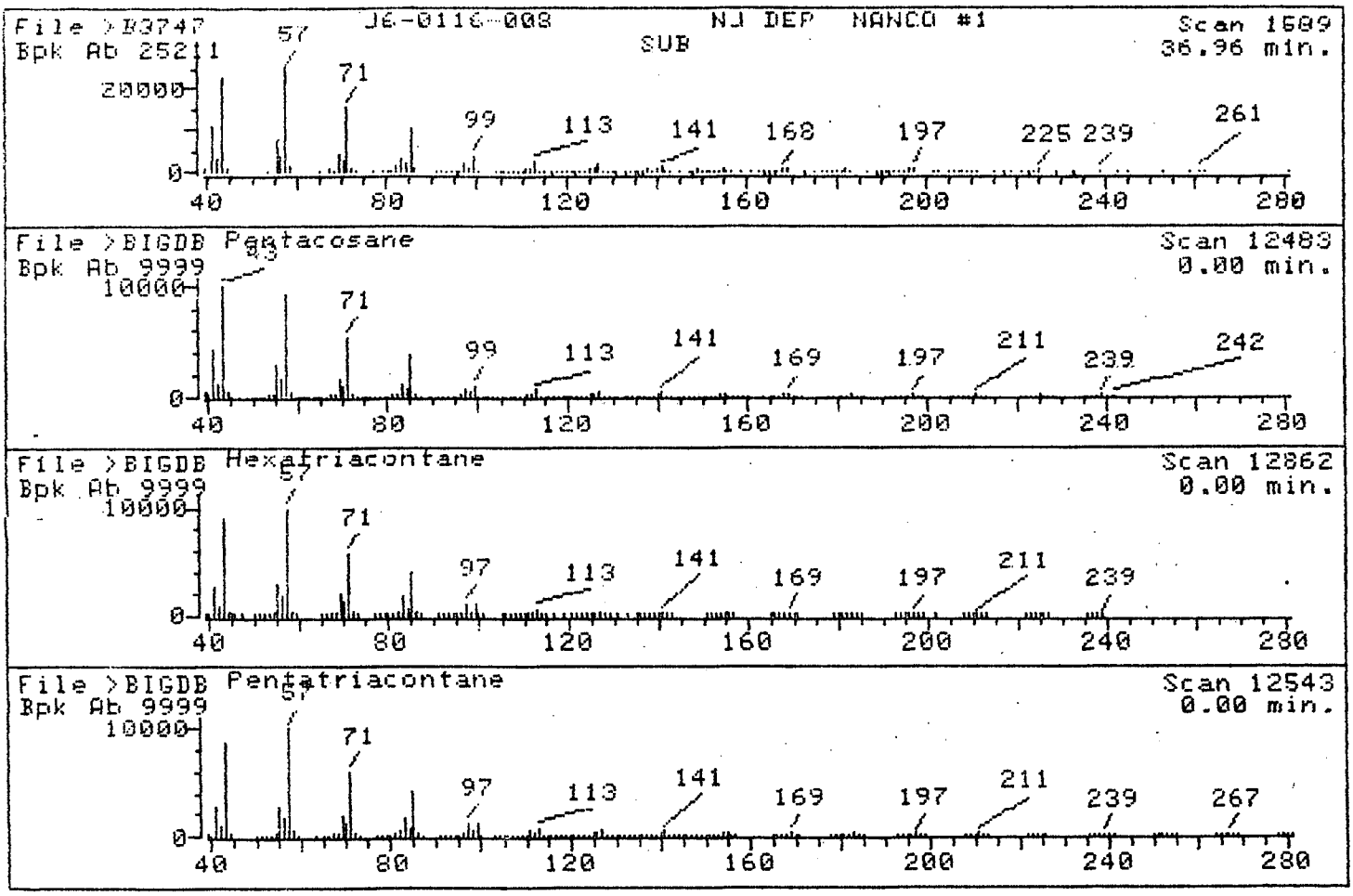


000324

1. 1,2-Benzenedicarboxylic acid, dinonyl ester 418 C26H4204
2. 1,2-Benzenedicarboxylic acid, diisooctyl ester 390 C24H3804
3. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) este 390 C24H3804
4. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) este 390 C24H3804
5. 1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) este 390 C24H3804

Sample file: >B3747 Spectrum #: 1569
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	36	84764	36508	"BIGDB	62	96	2	0	64	30	14	13
2.	28	27554263	36389	"BIGDB	66	78	2	0	71	39	10	14
3.	25	414	249	PRIPOL	57	83	1	0	71	46	7	15
4.	25	117817	36500	"BIGDB	57	83	1	0	71	46	7	15
5.	20	117817	36501	"BIGDB	37	37	2	0	81	52	5	12

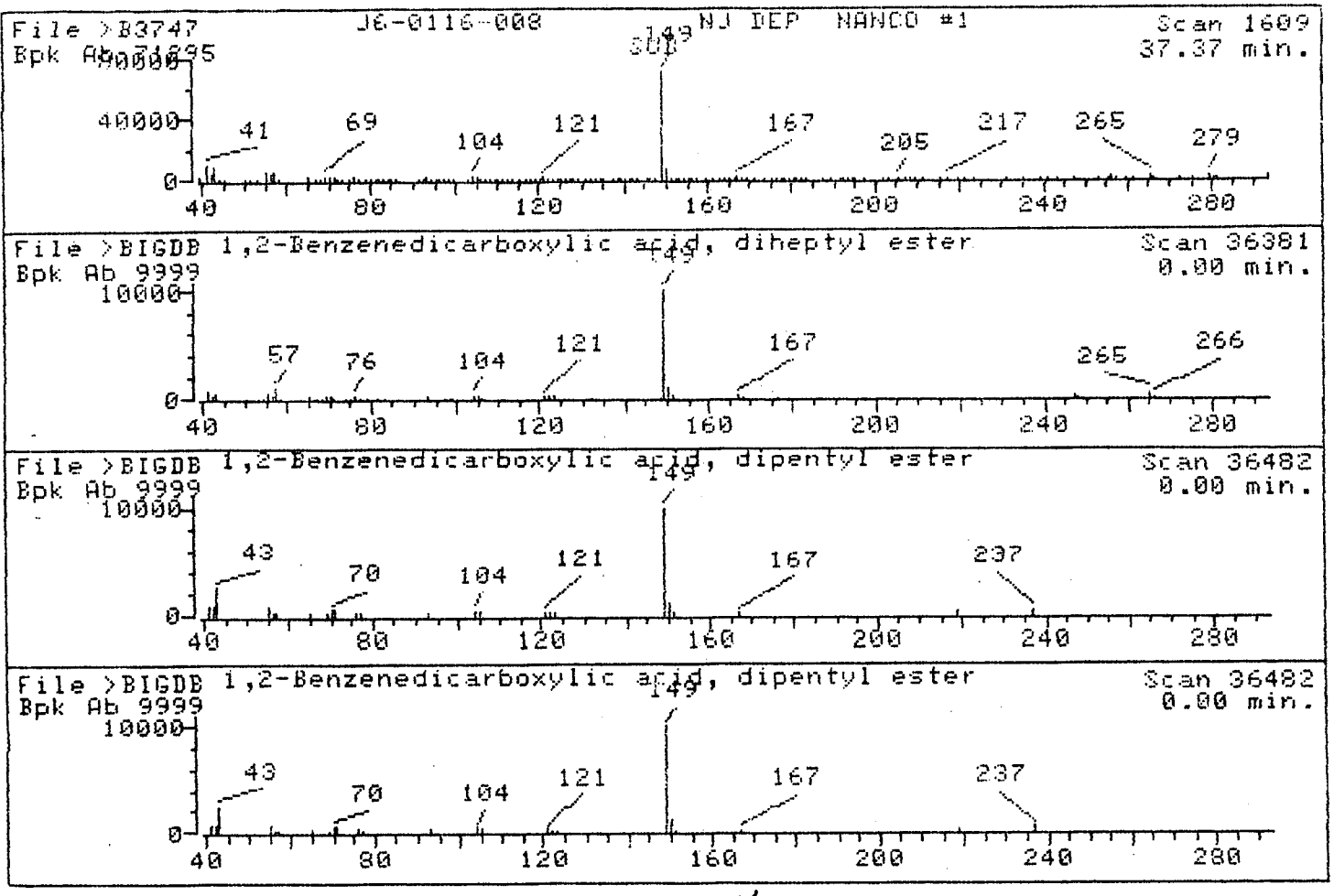


000325

1.	Pentacosane	352	C25H52
2.	Hexatriacontane	506	C36H74
3.	Pentatriacontane	492	C35H72
4.	Hexatriacontane	506	C36H74
5.	Octadecane	254	C18H38

Sample file: >B3747 Spectrum #: 1589
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89	629992	12483	"BIGDB	126	18	0	0	89	6	62	86
2.	89	630068	12862	"BIGDB	118	35	0	0	72	8	62	80
3.	89	630079	12543	"BIGDB	117	34	0	0	67	6	62	80
4.	88	630068	12864	"BIGDB	118	44	2	0	72	5	65	57
5.	88	593453	12397	"BIGDB	92	28	1	0	83	5	65	50



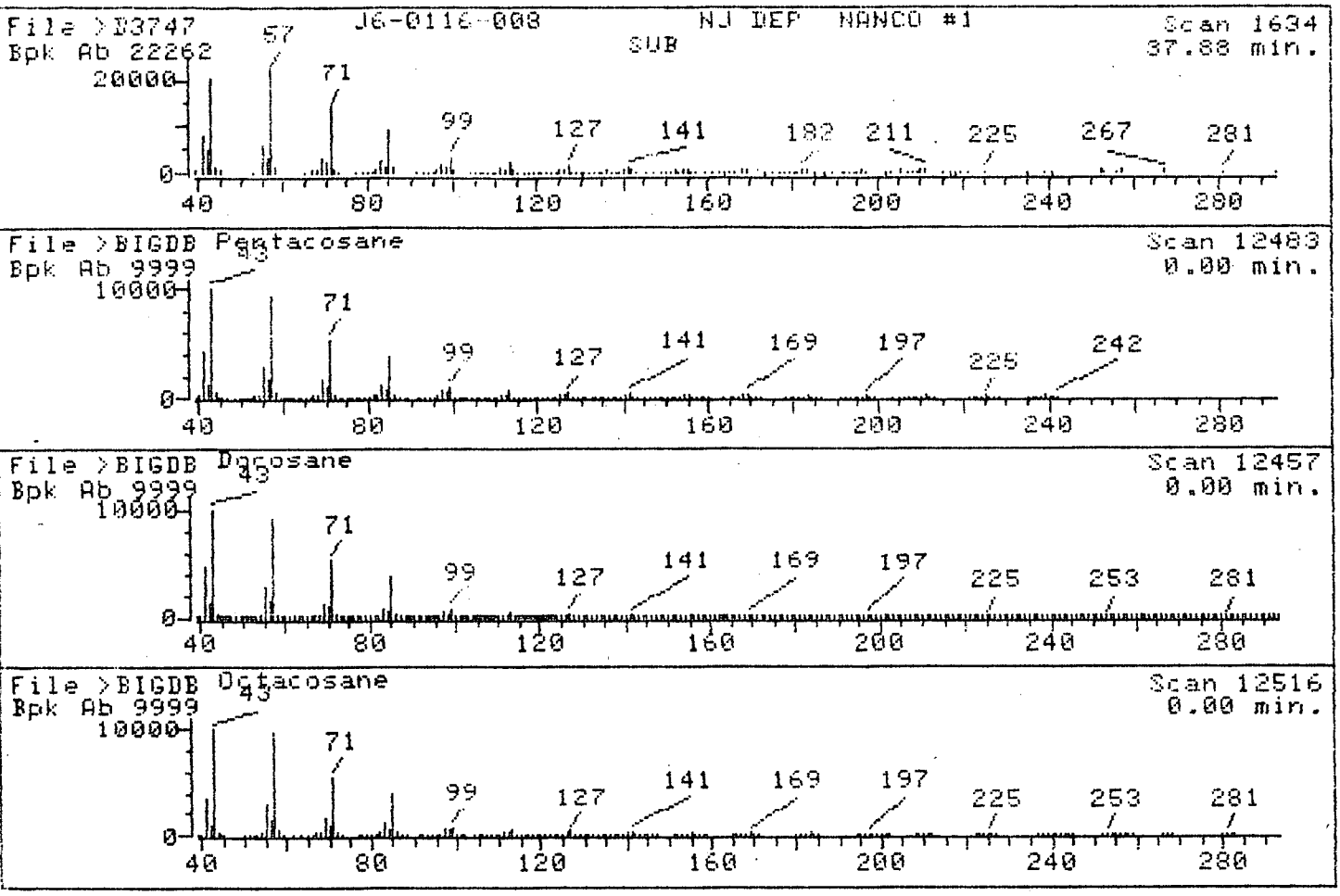
Dimroth Photo 1/96

000326

1. 1,2-Benzenedicarboxylic acid, diheptyl ester 362 C22H3404
2. 1,2-Benzenedicarboxylic acid, dipentyl ester 306 C18H2604

Sample file: >B3747 Spectrum #: 1609
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	35	3648213	36381	"BIGDB	79	39	1	0	58	50	11	31
2.	20	131180	36482	"BIGDB	37	53	1	0	43	54	5	13

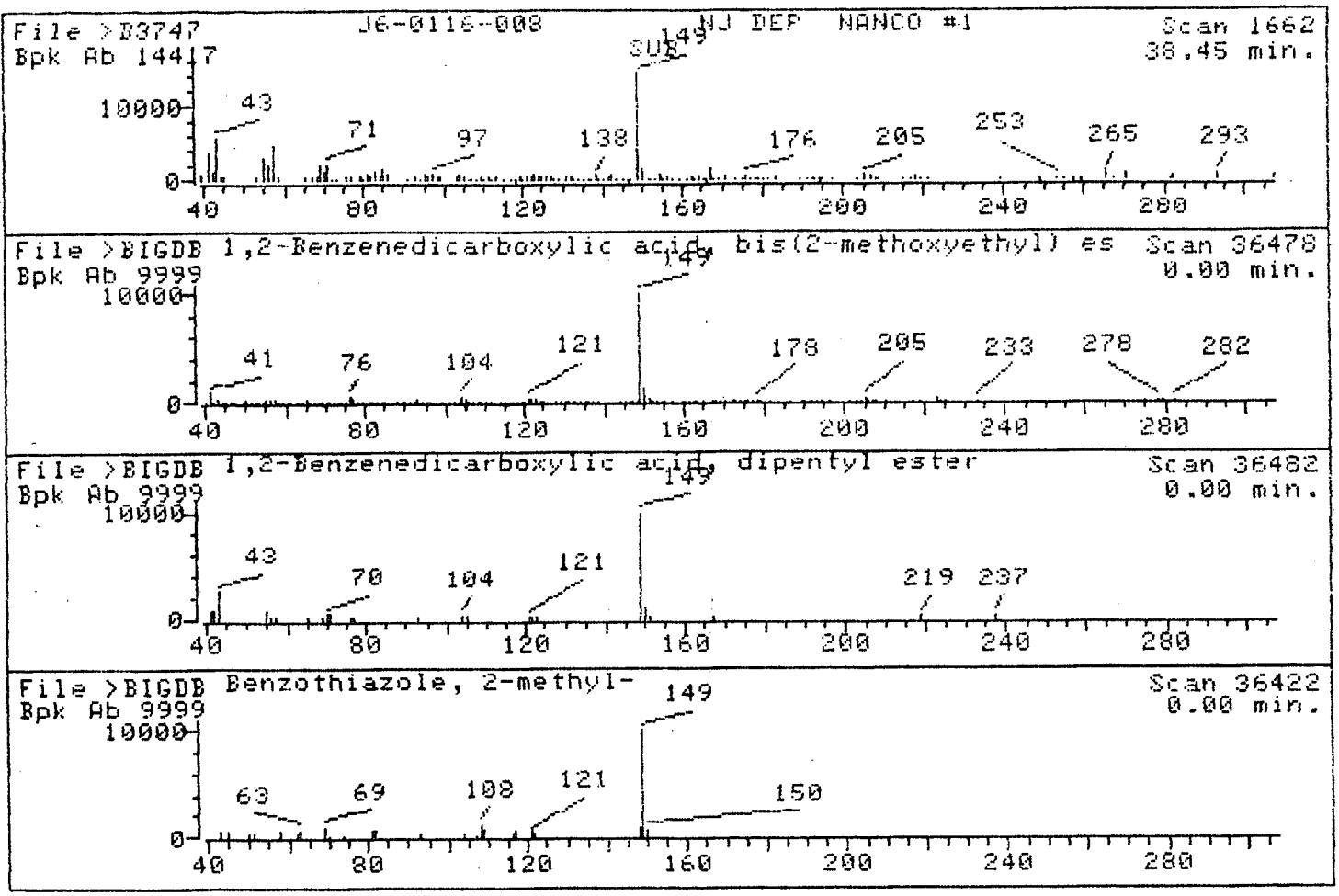


000327

1.	Pentacosane	352	C25H52
2.	Docosane	310	C22H46
3.	Octacosane	394	C28H58
4.	Heneicosane	296	C21H44
5.	Dotriacontane	450	C32H66

Sample file: >B3747 Spectrum #: 1634
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89	629992	12483	"BIGDB	124	20	0	0	84	8	62	86
2.	84	629970	12457	"BIGDB	111	21	1	0	91	8	55	69
3.	84	630024	12516	"BIGDB	113	24	1	0	91	8	55	69
4.	84	629947	12449	"BIGDB	106	21	1	0	91	10	55	66
5.	84	544854	12534	"BIGDB	120	37	2	0	72	10	55	60

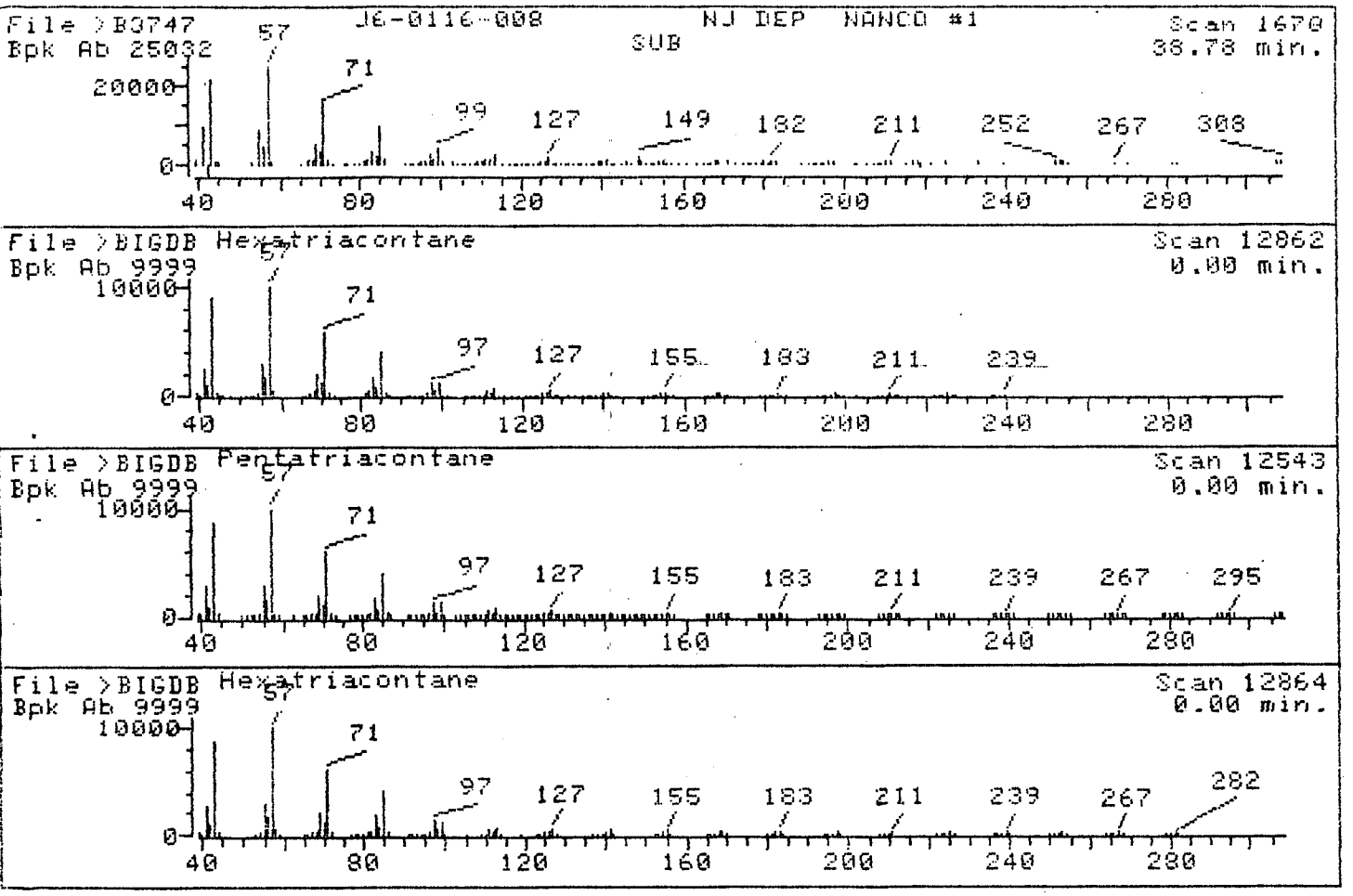


000328

1. 1,2-Benzenedicarboxylic acid, bis(2-methoxyethyl) es ter — 282 C14H1806
2. 1,2-Benzenedicarboxylic acid, dipentyl ester — 306 C18H2604
3. Benzothiazole, 2-methyl- — 149 C8H7NS
4. 1,2-Benzenedicarboxylic acid, diisodecyl ester — 446 C28H4604
5. PHENYL(I-P-DIPHENYLMETHYLPHENYL-3,3-DIMETHYL)BUTYL K ETONE — 432 C32H320

Sample file: >B3747 Spectrum #: 1662
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	43*	117828	36478	"BIGDB	29	73	2	0	90	23	17	14
2.	39	131180	36482	"BIGDB	58	54	1	0	80	27	14	16
3.	36*	120752	36422	"BIGDB	26	64	3	0	100	29	14	13
4.	25	26761400	36410	"BIGDB	66	83	2	0	57	50	7	14
5.	20	0	36405	"BIGDB	47	45	2	0	55	52	5	14

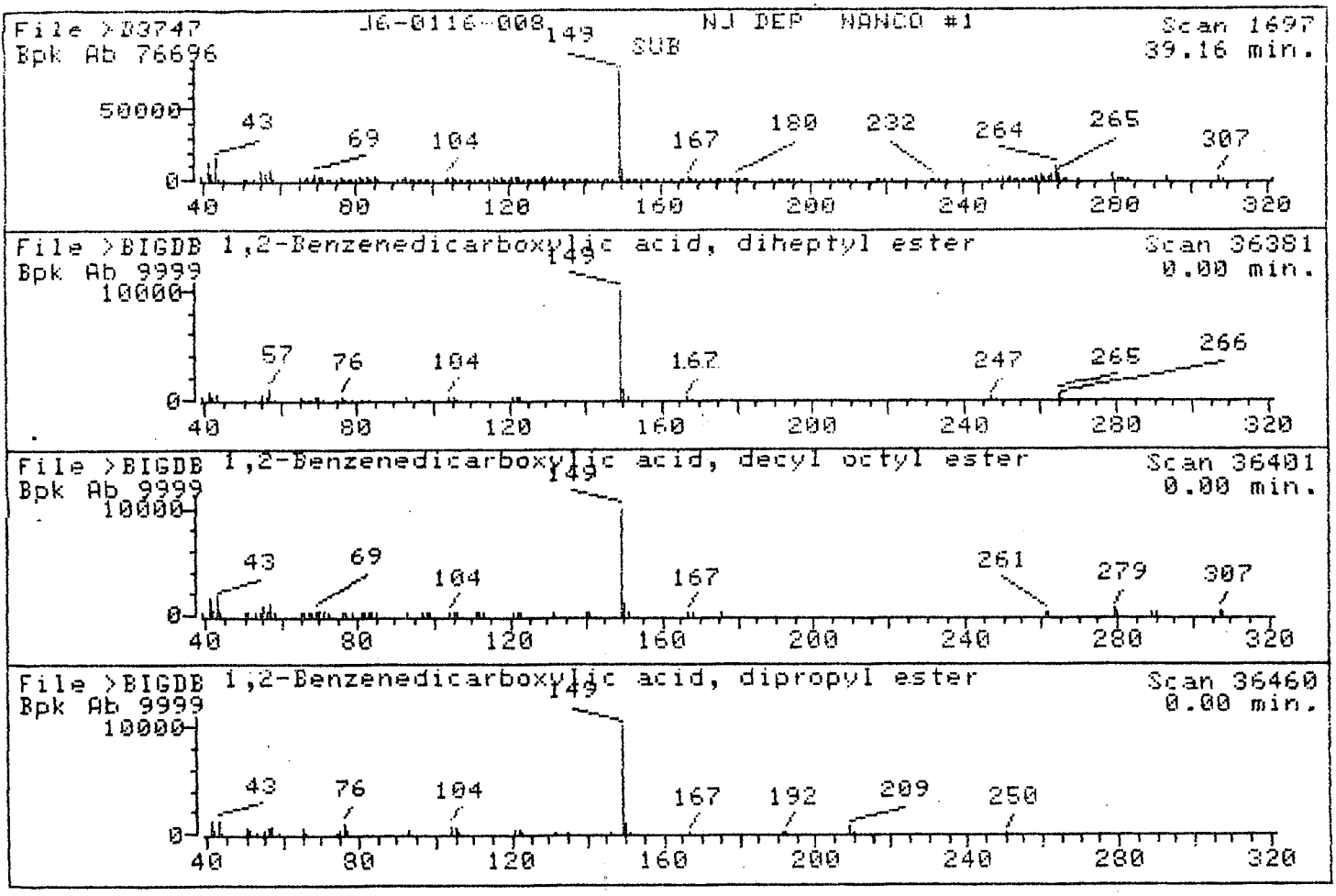


000359

1. Hexatriacontane 506 C36H74
2. Pentatriacontane 492 C35H72
3. Hexatriacontane 506 C36H74
4. Docosane, 11-butyl- 366 C26H54
5. Docosane, 11-decyl- 450 C32H66

Sample file: >B3747 Spectrum #: 1678
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	94	630068	12862	"BIGDB	135	18	0	0	76	7	68	93
2.	89	630079	12543	"BIGDB	134	17	1	0	77	7	62	83
3.	89	630068	12864	"BIGDB	120	42	2	0	69	5	66	60
4.	88	13475768	12836	"BIGDB	115	36	2	0	88	5	65	55
5.	87	55401553	12857	"BIGDB	111	46	2	0	77	5	63	49

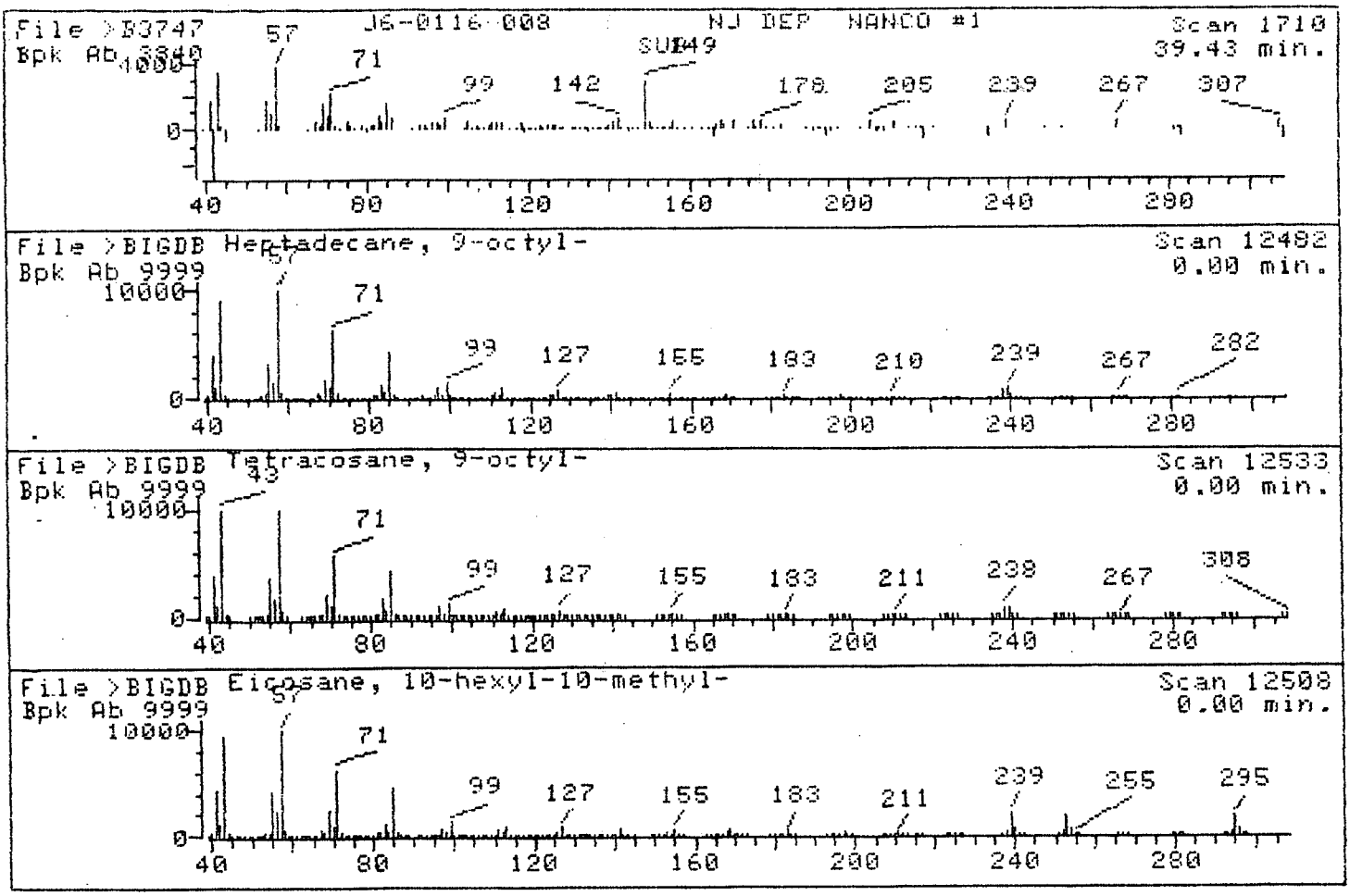


000330

1. 1,2-Benzenedicarboxylic acid, diheptyl ester 362 C22H3404
2. 1,2-Benzenedicarboxylic acid, decyl octyl ester 418 C26H4204
3. 1,2-Benzenedicarboxylic acid, dipropyl ester 250 C14H1804
4. 1,2-Benzenedicarboxylic acid, dipropyl ester 250 C14H1804
5. 1,2-Benzenedicarboxylic acid, bis(1-methylheptyl) es ter 390 C24H3804

Sample file: >B3747 Spectrum #: 1697
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	59	3648213	36381	"BIGDB	84	34	1	0	75	24	27	38
2.	44	119073	36401	"BIGDB	106	23	1	0	66	54	11	66
3.	37*	131168	36460	"BIGDB	31	78	2	0	100	28	14	14
4.	37*	131168	36310	"BIGDB	25	81	2	0	99	28	14	14
5.	37	131157	36392	"BIGDB	64	60	2	0	94	26	14	14

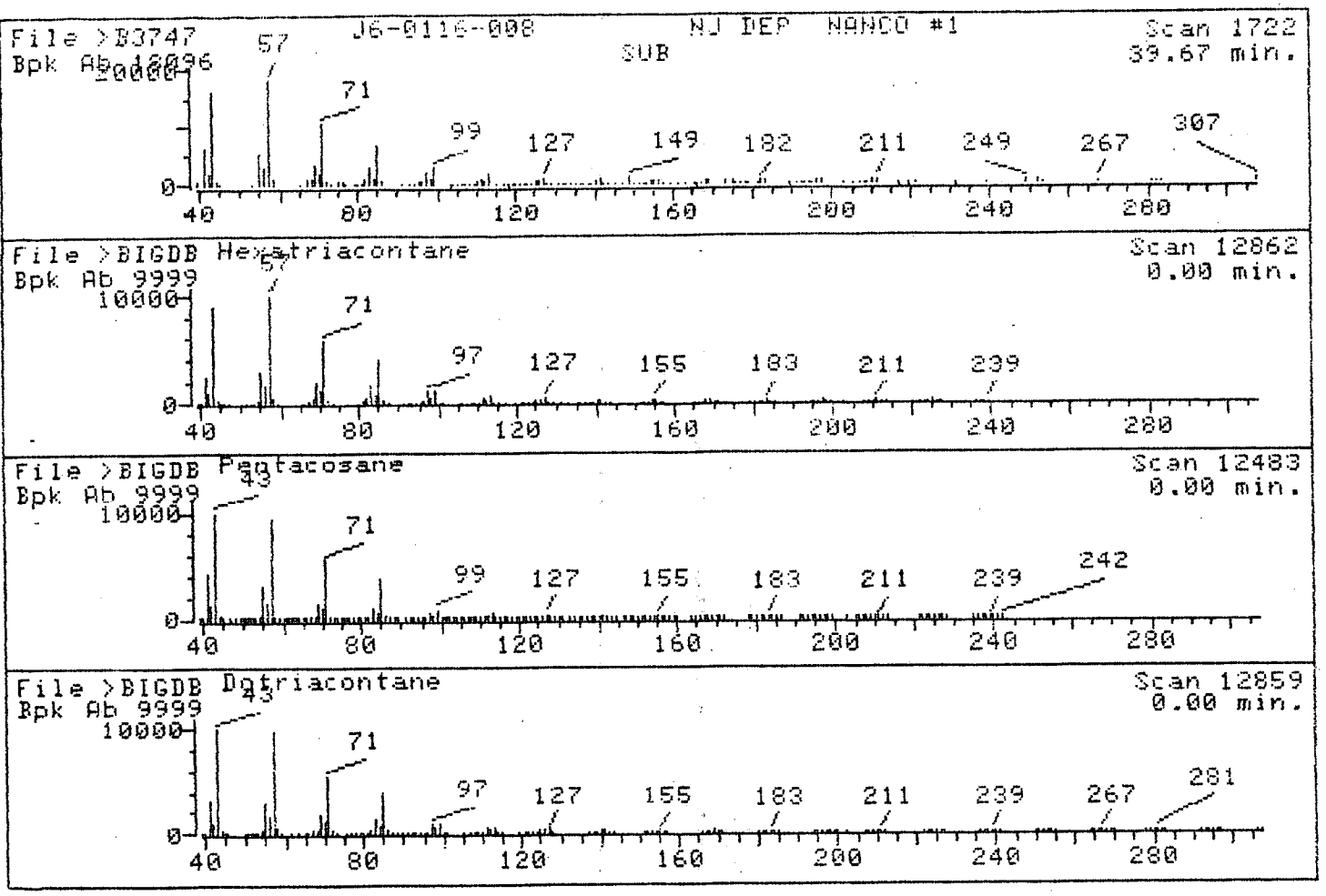


0:0361

1. Heptadecane, 9-octyl-	352	C25H52
2. Tetracosane, 9-octyl-	450	C32H66
3. Eicosane, 10-hexyl-10-methyl-	380	C27H56
4. 2,6-NONANEDIONE	156	C9H16O2
5. 2-N-PENTYLBENZOTHIAZOLE	205	C12H15NS

Sample file: >B3747 Spectrum #: 1710
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	18	7225641	12482	"BIGDB	79	64	2	0	89	60	4	21
2.	15	55401542	12533	"BIGDB	73	89	3	0	89	60	3	13
3.	15	55282321	12508	"BIGDB	71	91	3	0	85	60	3	12
4.	15*	0	12092	"BIGDB	30	66	2	0	89	60	3	14
5.	15*	0	36246	"BIGDB	23	60	3	0	76	60	3	12

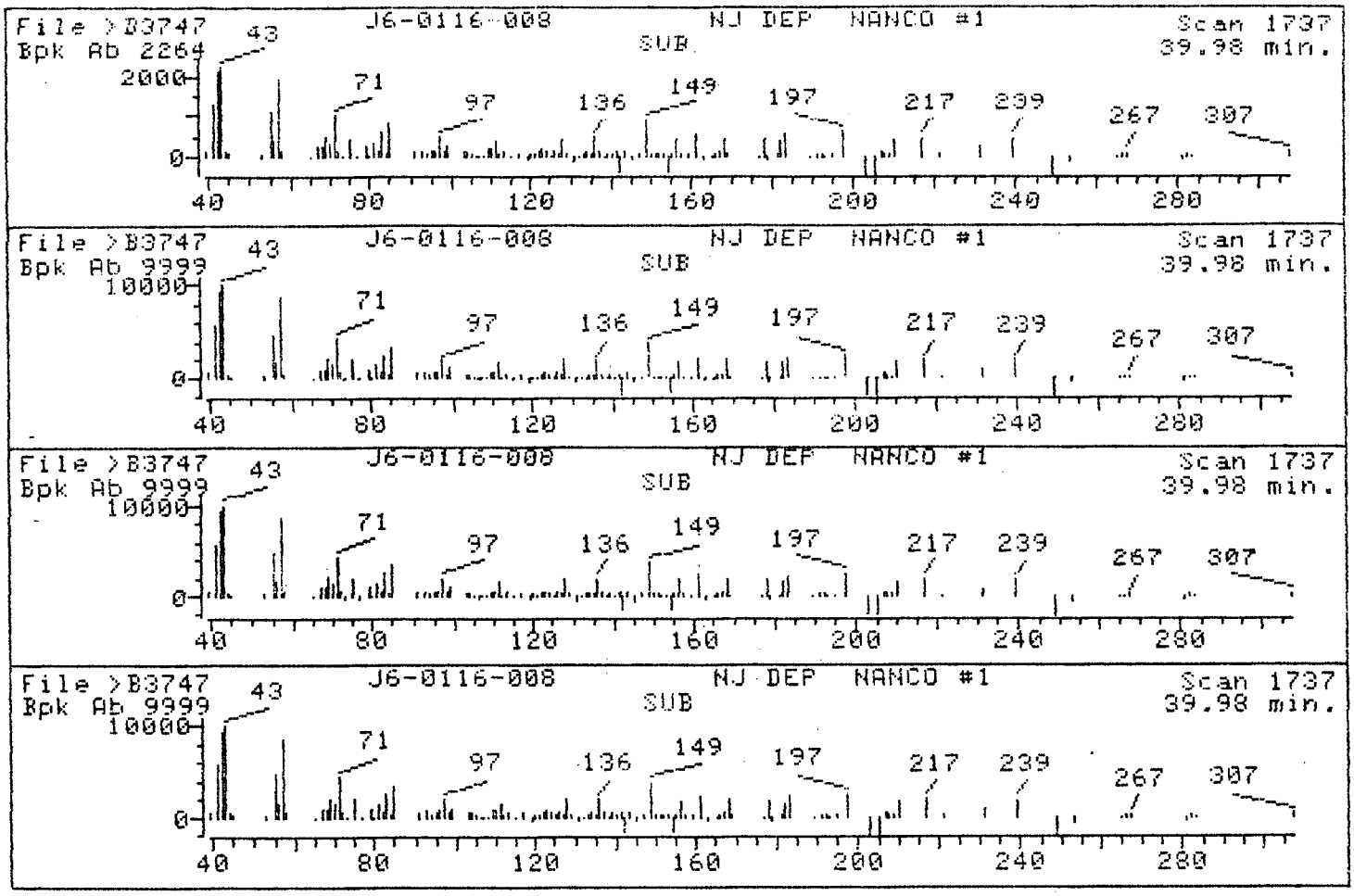


000832

1. Hexatriacontane 506 C36H74
2. Pentacosane 352 C25H52
3. Dotriacontane 450 C32H66
4. Octacosane 394 C28H58
5. Pentatriacontane 492 C35H72

Sample file: >B3747 Spectrum #: 1722
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	93	630068	12862	"BIGDB	137	16	1	0	88	4	68	86
2.	89	629992	12483	"BIGDB	126	18	1	0	85	4	66	77
3.	89	544854	12859	"BIGDB	123	28	1	0	88	4	66	76
4.	89	630024	12516	"BIGDB	113	24	1	0	88	4	66	69
5.	89	630079	12543	"BIGDB	117	34	1	0	80	4	66	72



01 0823

Sample file: >B3747 Spectrum #: 1737

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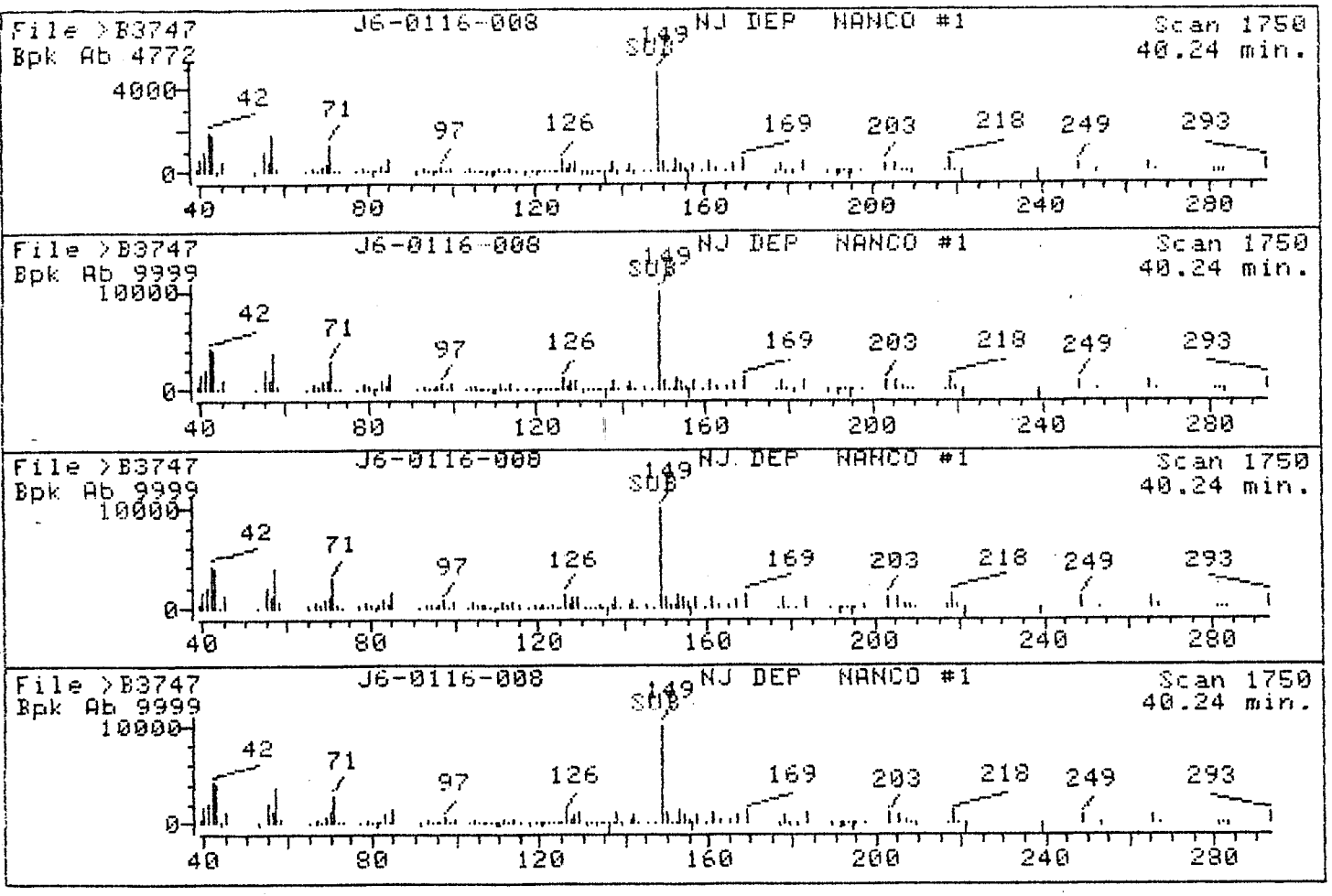

000334

Sample file: >B3747 Spectrum #: 1750

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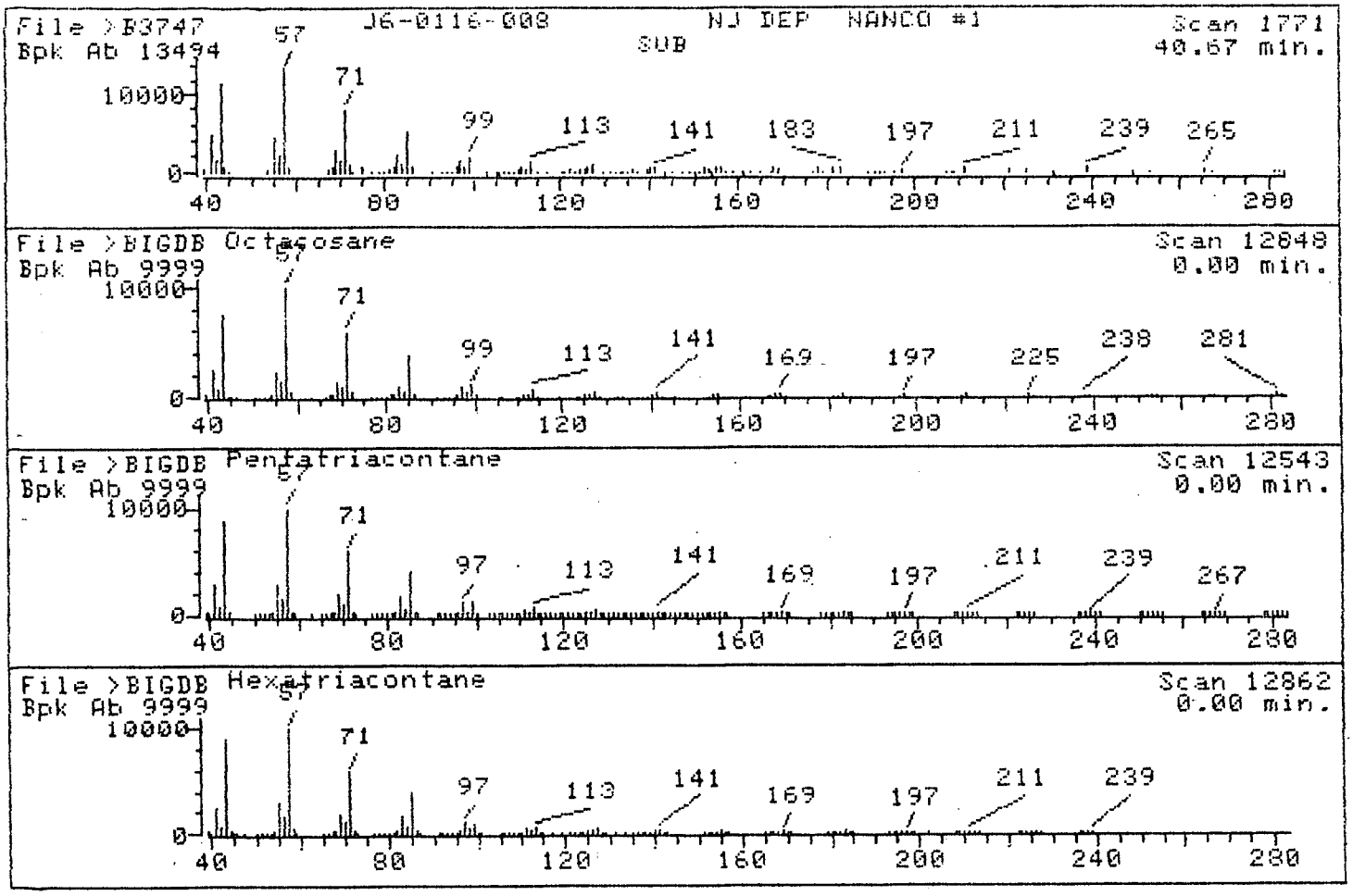
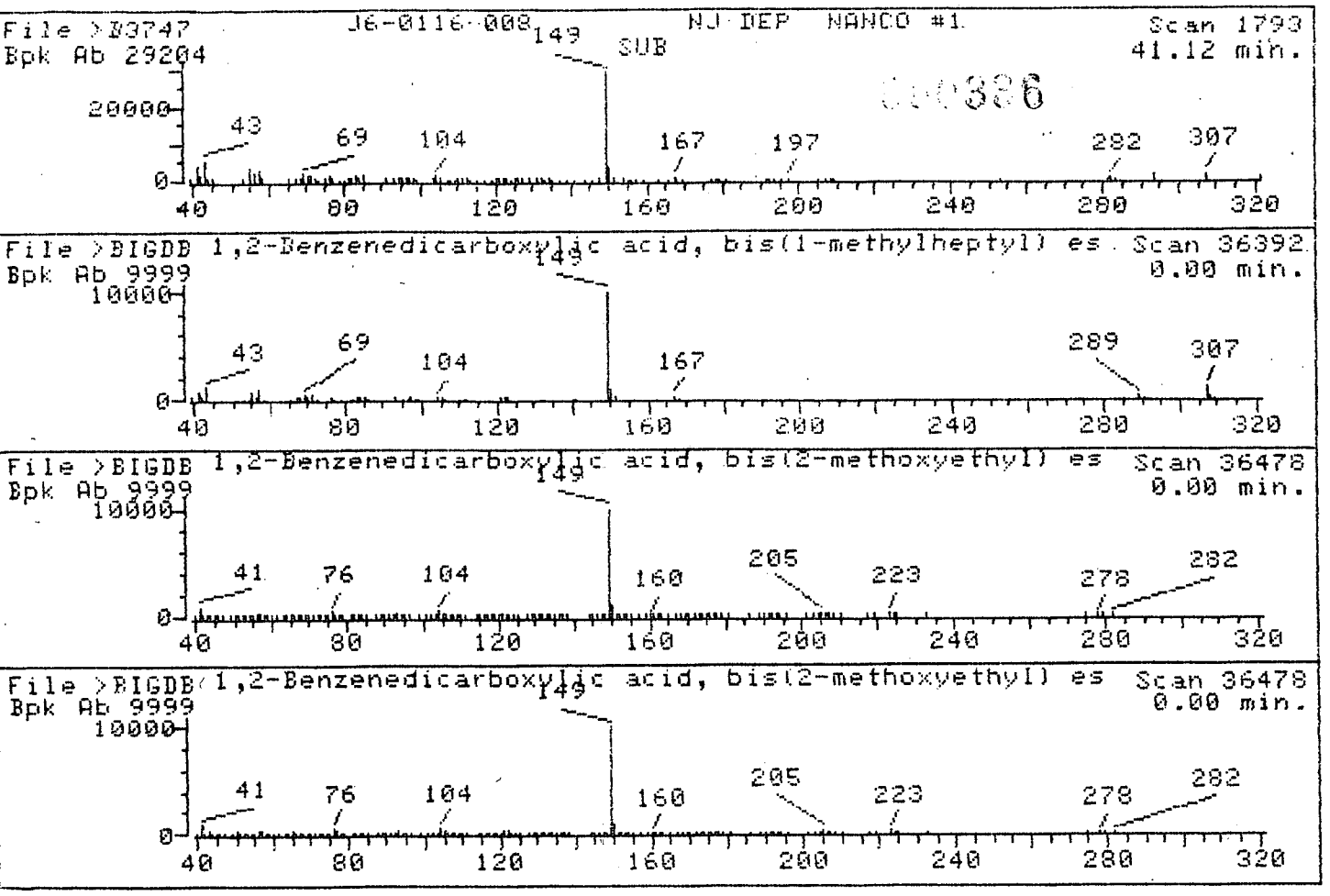


000085

1. Octacosane	394	C28H58
2. Pentatriacontane	492	C35H72
3. Hexatriacontane	506	C36H74
4. Eicosane, 7-hexyl-	366	C26H54
5. Docosane, 7-hexyl-	394	C28H58

Sample file: >B3747 Spectrum #: 1771
Search speed: 1 Tilting option: N No. of ion ranges searched: 45

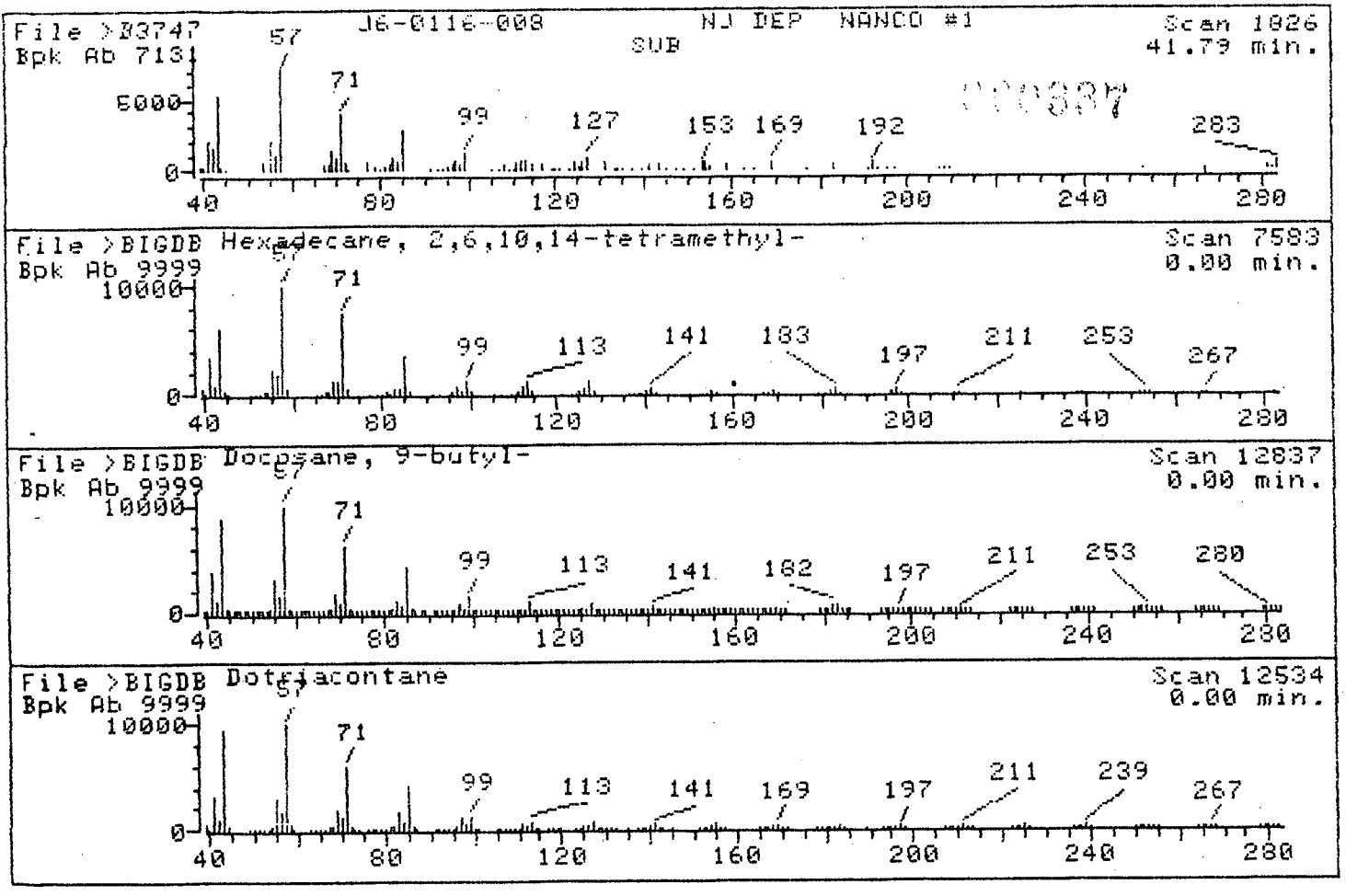
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89	630024	12848	"BIGDB	120	24	1	0	93	5	66	74
2.	89	630079	12543	"BIGDB	121	30	1	0	82	5	66	74
3.	89	630068	12862	"BIGDB	110	43	1	0	90	5	66	67
4.	88	55333998	12501	"BIGDB	112	33	2	0	89	4	65	50
5.	88	55373869	12515	"BIGDB	112	40	2	0	86	4	65	50



1. 1,2-Benzenedicarboxylic acid, bis(1-methylheptyl) es 390 C24H3804
   ter
2. 1,2-Benzenedicarboxylic acid, bis(2-methoxyethyl) es 282 C14H1806
   ter

Sample file: >B3747 Spectrum #: 1793
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	60	131157	36392	"BIGDB	65	59	2	0	97	11	30	14
2.	52*	117828	36478	"BIGDB	27	75	2	0	94	17	20	14



1.	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42
2.	Docosane, 9-butyl-	366	C26H54
3.	Dotriacontane	450	C32H66
4.	Hexadecane, 5-butyl-	282	C20H42
5.	Pentatriacontane	492	C35H72

Sample file: >B3747 Spectrum #: 1826
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	83*	638368	7583	"BIGDB	100	35	2	0	72	13	51	77
2.	79	55282149	12837	"BIGDB	103	48	2	0	84	10	48	37
3.	74	544854	12534	"BIGDB	107	50	2	0	74	15	39	44
4.	74*	6912078	12425	"BIGDB	75	68	3	0	73	13	39	40
5.	71	630079	12543	"BIGDB	102	49	2	0	71	15	38	36

NJ DEP BNA 10/22/86 1079

(~~moisture~~)

JB 3747 J6-0116-008

Naphthalene	3.3 J	ug/L
4-Chloraniline	15	
2-Meth naph	24	
2,4 Dinitro Tol	13	
Fluorene	10	
N-Nitroso diph. amin	53	
Phenanthrene	19	
bis(2 Eth hex)phth	77 B	
Di-n-oct phth	65	

SURR

Phenol-d5	32 %
2 Fl Phenol	36
Nitro benz.	74
2 Fl biph	80
Bromol	58
Terph	122

TIC's b = (40 x 2.22)/790072 = 0.000112394

unknown Hydrocarbon (17.036) cx = 2739150 xb = 310 J

" " (17.321) cx = 1106231 xb = 120 J

unknown polyaromatic Hydrocarbon (18.989) cx = 4972506 xb = 56 J

unknown Hydrocarbon (20.374) cx = 1140695 xb = 130 J

(629594) Tetradecane (20.802) cx = 8231371 xb = 920 J

Isomer of dimethyl naphthalene (21.251) cx = 1199117 xb = 130 J

unknown Hydrocarbons (21.597) cx = (2452272 xb) = 280 J

" " (21.842) cx = 2939943 xb = 330 J

" " (22.475) cx = 6626575 xb = 740 J

Continue → next pg

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Witn

Sohail Jaha 10/27/86

BNA NJDEP 10/22/86 1079

20
JB 3747 Con'd ~~at~~ J6-116-008 Con'd

TIC' con'd

isomer of naphthalene (23.332) cx = 1274685 xb = 140 J

(544763) Hexadecane (24.047) cx = 8481152 xb = 950 J

unknown (24.885) cx = 1819526 xb = 200 J

(629787) Heptadecane (25.518) cx = 7167990 xb = 800 J

(1921706) pentadecane, 2,6,10,14-tetramethyl- (25.600) cx = 4020726 xb = ~~4~~ 450

unknown Hydrocarbon (26.111) cx = (1306571) xb = 150 J

(638368) Hexadecane, 2,6,10,14-tetramethyl- (27.031) cx = 2891976 xb = ~~37~~ 320

unknown Hydrocarbons (27.440) cx = (851249 xb) = 96 J

" " (28.217) cx = 5186672 xb = 580 J

" " (29.464) cx = (3907901) xb = 440 J

" " (29.934) cx = (985335 xb) = 110 J

" " (30.670) cx = 2611468 xb = 290 J

" " (31.120) cx = 1025952 xb = 110 J

" " (31.815) cx = 2094153 xb = 240 J

" " (32.915) cx = 1126620 xb = 130 J

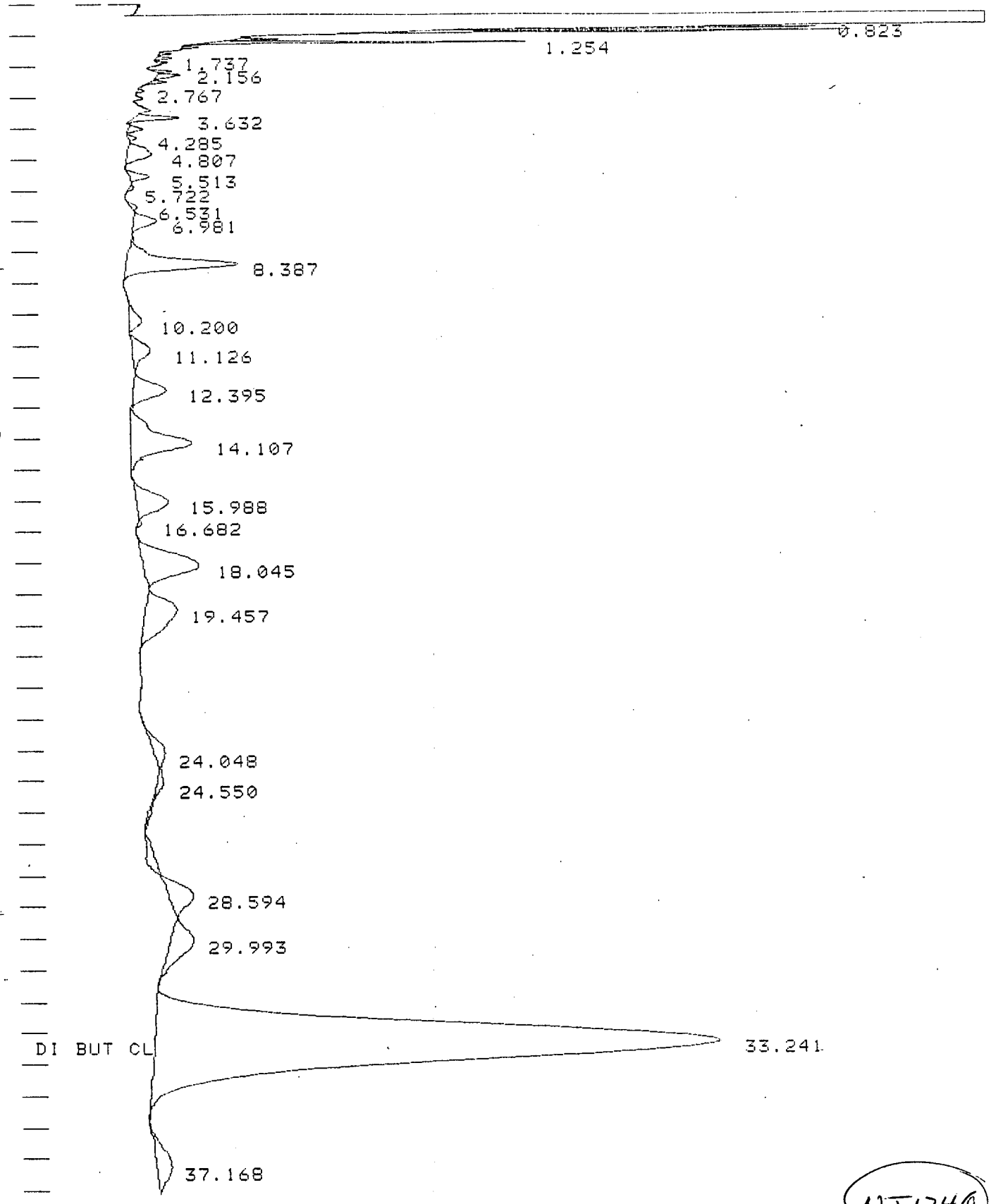
Witness

Sohal Soh 10/27/86

7

000340

CHART SPEED 0.6 CM/MIN
ATTEN: 4 ZERO: 5% 1 MIN/TICK



varian /sunnyvale, calif. p/n 03-906362-01

Sw 2

NJ1746

SW 2 (N51746)

TITLE: PESTICIDE & PCB ANALYSIS 0:35 2 OCT 86

CHANNEL NO: 2 SAMPLE: J6-0116-008 METHOD: PEST4Q

PEAK NO	PEAK NAME	RESULT %	TIME (MIN)	TIME OFFSET	AREA COUNTS	RRT	SEP CODE	W1/2 (SEC)
1		0.6282	0.823		1949	0.03	BB	1.45
2		1.4955	0.920		4640	0.03	BB	1.95
3		0.1460	1.161		453	0.03	BB	2.35
4		1.2631	1.254		3919	0.04	BB	2.50
5		0.0741	1.396		230	0.04	T	2.95
6		0.1028	1.737		319	0.05	BB	4.20
7		0.0938	2.156		291	0.06	BB	4.65
8		0.2227	2.278		691	0.07	BB	8.90
9		0.1041	2.498		323	0.08	BB	5.80
10		0.5344	3.632		1658	0.11	BB	? 7.45
11		0.2069	3.996		642	0.12	BB	9.20
12		0.1057	4.285		328	0.13	BB	8.20
13		0.9073	4.807		2815	0.14	BB	11.60
14		0.4035	5.513		1252	0.17	BB	? 13.50
15		0.0793	5.722		246	0.17	BB	? 33.10
16		0.0989	6.531		307	0.20	BB	? 14.10
17		0.7371	6.981		2287	0.21	BB	24.80
18		3.8903	8.387		12070	0.25	BB	19.80
19		0.5221	10.200		1620	0.31	BB	? 27.25
20		0.9560	11.126		2966	0.33	BB	24.00
21		1.5442	12.395		4791	0.37	BB	33.05
22		3.7417	14.107		11609	0.42	BB	34.65
23		1.8223	15.988		5654	0.48	BB	40.60
24		3.8661	18.045		11995	0.54	BB	? 52.15
25		2.8863	19.457		8955	0.58	BB	? 77.45
26		0.7835	24.048		2431	0.72	BB	? 72.70
27		0.1818	24.550		564	0.74	BB	?140.30
28		1.0733	28.594		3330	0.86	BB	? 67.40
29		2.0538	29.993		6372	0.90	BB	?113.35
30	DI BUT CL	68.0140	33.241	0.181	211021	1.00	VV	78.05
31		1.4610	37.168		4533	1.12	T	? 93.90
TOTALS:		99.9998		0.181	310261			

DETECTED PKS: 37 REJECTED PKS: 6

MULTIPLIER: 1.00000

NOISE: 18.2 OFFSET: -46

RACK: 8 VIAL: 1 INJ: 1

SAVED FILE: PEST4Q012

NOTES:
***** NANCO LABS, INC *****
1.95%SP2401+1.5%SP2250 ON 100/120 SUPEL.
LENGTH:2.0M; OD:1/4"; ID:2MM; GLASS
INJ @ 200°C;DET @ 250°C; ECD RANGE: 10
OVEN: 192°C ISOTHERMAL; UL INJECTED:3.0
GC: VARIAN 3700 #2; MODEL #371116-00
CARRIER GAS: 95%AR+5%ME @ 22ML/MIN
ANALYST: S. EASTER

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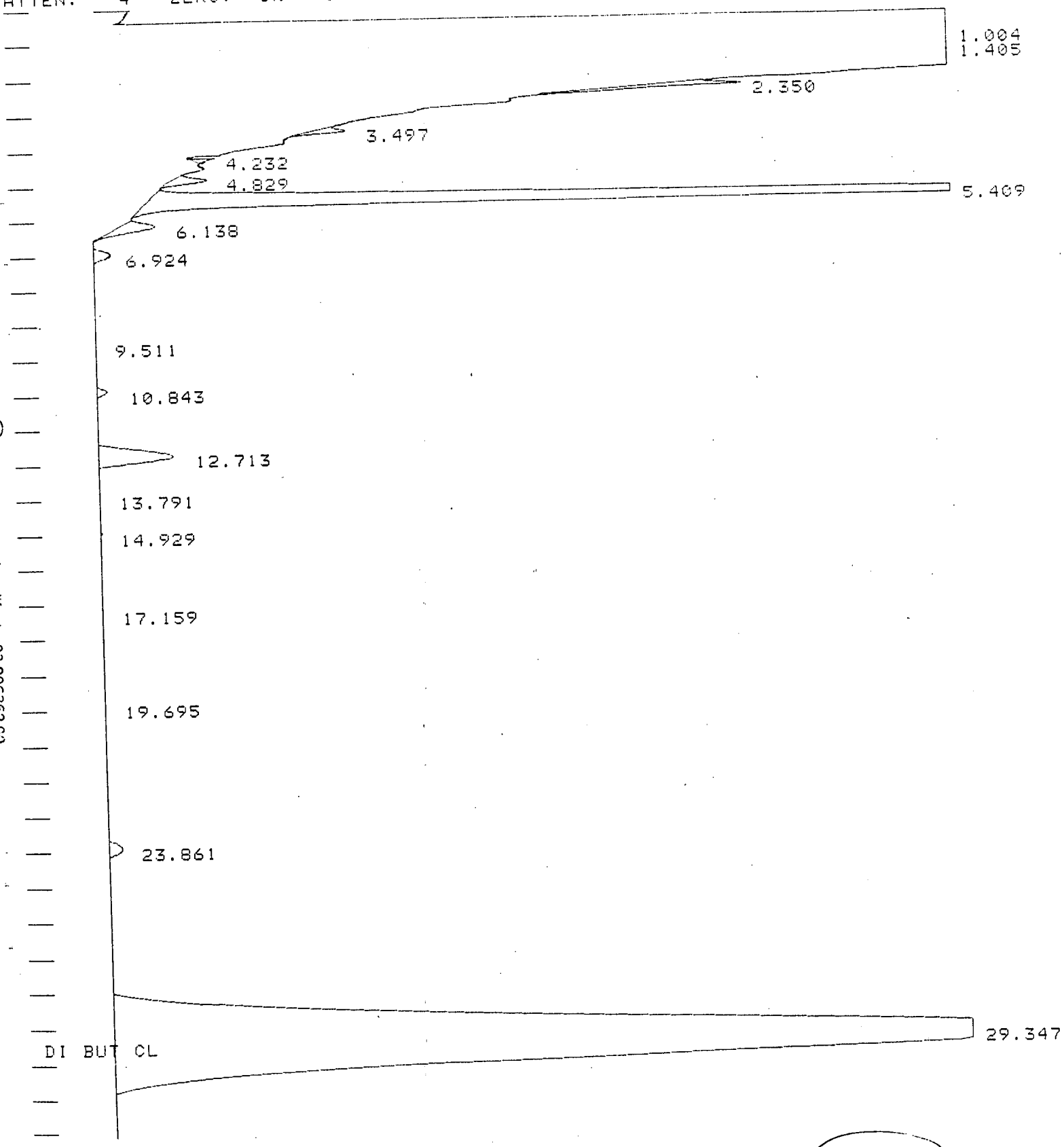
CU0362

CHART SPEED 0.7 CM/MIN
ATTEN: 4 ZERO: 5% 1 MIN/TICK



varian /sunnyvale, calif. p/n 03-906362-00

SW 2

NJ184C

SW 2 (NJ184C)

TITLE: PESTICIDE & PCB ANALYSIS 15:50 1 OCT 86

CHANNEL NO: 1 SAMPLE: J6-0116-008 METHOD: PEST4C

PEAK NO	PEAK NAME	RESULT %	TIME (MIN)	TIME OFFSET	AREA COUNTS	RRT	SEP CODE	W1/2 (SEC)
1		0.7165	1.004		4284	0.03	BB	1.75
2		0.8267	1.405		4943	0.05	BB	2.75
3		0.4230	2.350		2529	0.08	BB	3.50
4		0.1693	3.497		1012	0.12	BB	4.70
5		0.3002	4.829		1795	0.16	BB	? 8.30
6		18.6463	5.409		111491	0.18	BB	11.90
7		0.4552	6.138		2722	0.21	BB	11.60
8		0.8175	6.924		4888	0.24	BB	? 16.30
9		0.1806	9.511		1080	0.32	BB	15.50
10		0.9697	10.843		5798	0.37	BB	? 26.00
11		2.4515	12.713		14658	0.43	BB	? 27.95
12		0.1509	13.791		902	0.47	BB	? 30.40
13		1.1393	14.929		6812	0.51	BB	36.75
14		1.4490	17.159		8664	0.58	BB	42.65
15		0.7688	19.695		4597	0.67	BB	42.65
16		3.6859	23.861		22039	0.81	BB	57.05
17	DI BUT CL	66.8497	29.347	0.327	399712	1.00	BB	71.25
TOTALS:		100.0000		0.327	597926			

DETECTED PKS: 18 REJECTED PKS: 1

MULTIPLIER: 1.00000

NOISE: 24.3 OFFSET: -19

RACK: 2 VIAL: 3 INJ: 1

SAVED FILE: PEST4C011

NOTES:
***** NANCO LABS, INC *****
3% SP2100 ON 100/120 SUPELCOPORT
LENGTH:2.0M; OD:1/4"; ID:2MM; GLASS
INJ @ 200°C;DET @ 250°C; ECD RANGE: 10
OVEN: 192°C ISOTHERMAL; UL INJECTED: 3.0
GC: VARIAN 3700 #2; MODEL #371116-00
CARRIER GAS: 95%AR+5%ME @ 30ML/MIN
ANALYST: S. EASTER

varian /sunnyvale, calif p/n 03-906362-00