Original

Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 17 08:12:17 2002 Quant Results File: SCAN508.RES

Will be re-ext

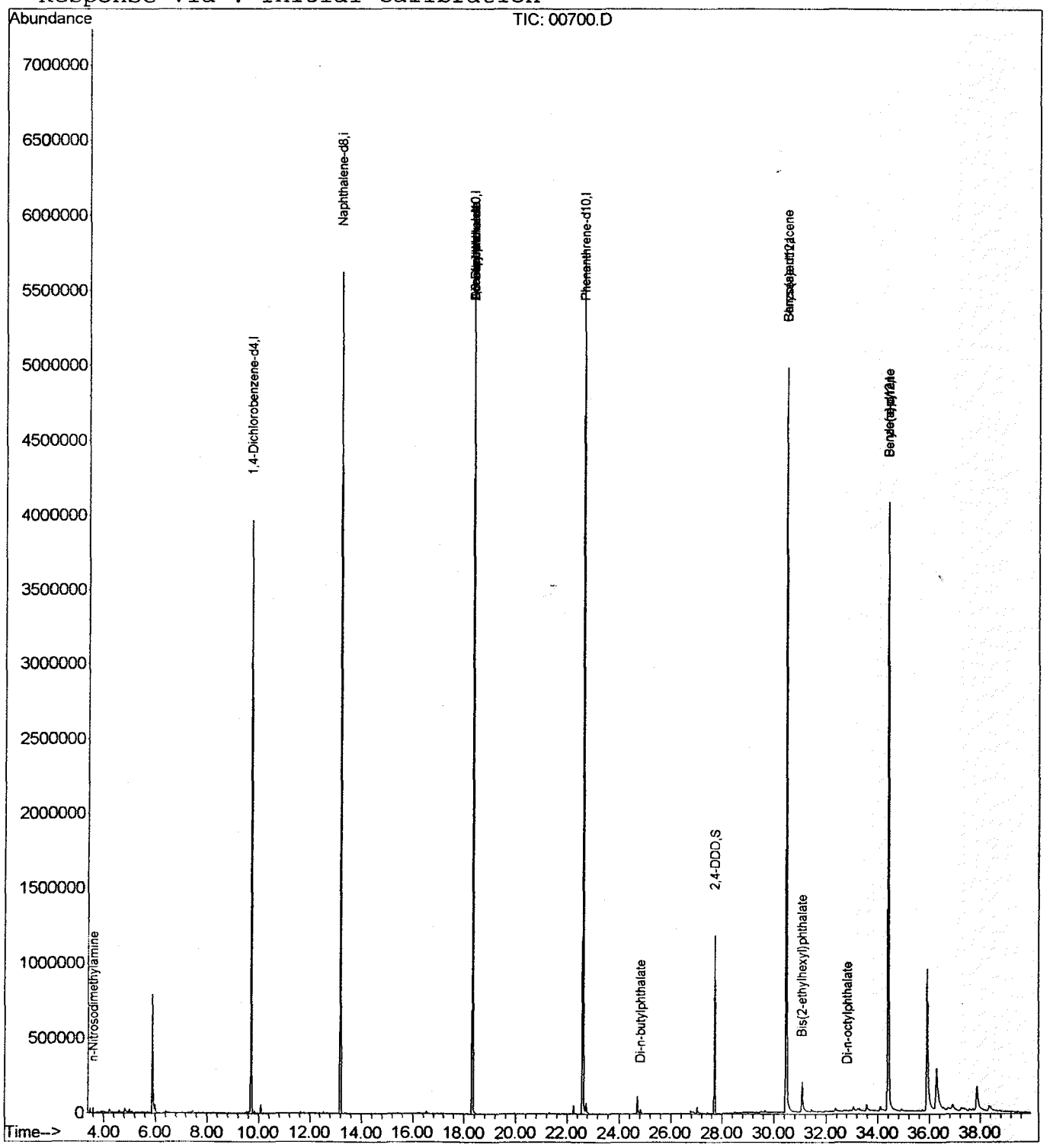
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Fri Jan 11 13:20:07 2002
Response via : Initial Calibration
DataAcq Meth : SCAN508

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1290915	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	5524078	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	2951497	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	4919254	20.00	ug/L	-0.02
38) Chrysene-d12	30.50	240	4262076	20.00	ug/L	-0.01
44) Perylene-d12	34.42	264	3074544	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	435285	5.60	ug/L	0.00
Spiked Amount 5.000			Recovery =	112.00%		
Target Compounds						Qvalue
2) n-Nitrosodimethylamine	3.60	74	10474	0.19	ug/L #	9
20) Dimethylphthalate	18.34	163	472767	2.43	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	375396	9.87	ug/L #	17
35) Di-n-butylphthalate	24.85	149	28686	0.09	ug/L	98
41) Benzo(a)anthracene	30.50	228	10408	0.04	ug/L #	58
42) Bis(2-ethylhexyl)phthalate	31.11	149	187171	1.43	ug/L	98
43) Chrysene	30.50	228	10408	0.04	ug/L #	56
45) Di-n-octylphthalate	32.84	149	6960	0.02	ug/L #	74
48) Benzo(a)pyrene	34.42	252	10415	0.05	ug/L #	1

(#) = qualifier out of range (m) = manual integration
00700.D SCAN508.M Thu Jan 17 08:12:17 2002 Page 1

Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Jan 17 8:12 2002 Quant Results File: SCAN508.RE

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title : 508 scan method
Last Update : Fri Jan 11 13:20:07 2002
Response via : Initial Calibration



LSC Area Percent Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Method : C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title : 508 scan method
Smoothing : OFF Filtering: 5
Sampling : 2 Min Area: 100 Area counts
Start Thrs: 0.2 Max Peaks: 20
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Signal : TIC

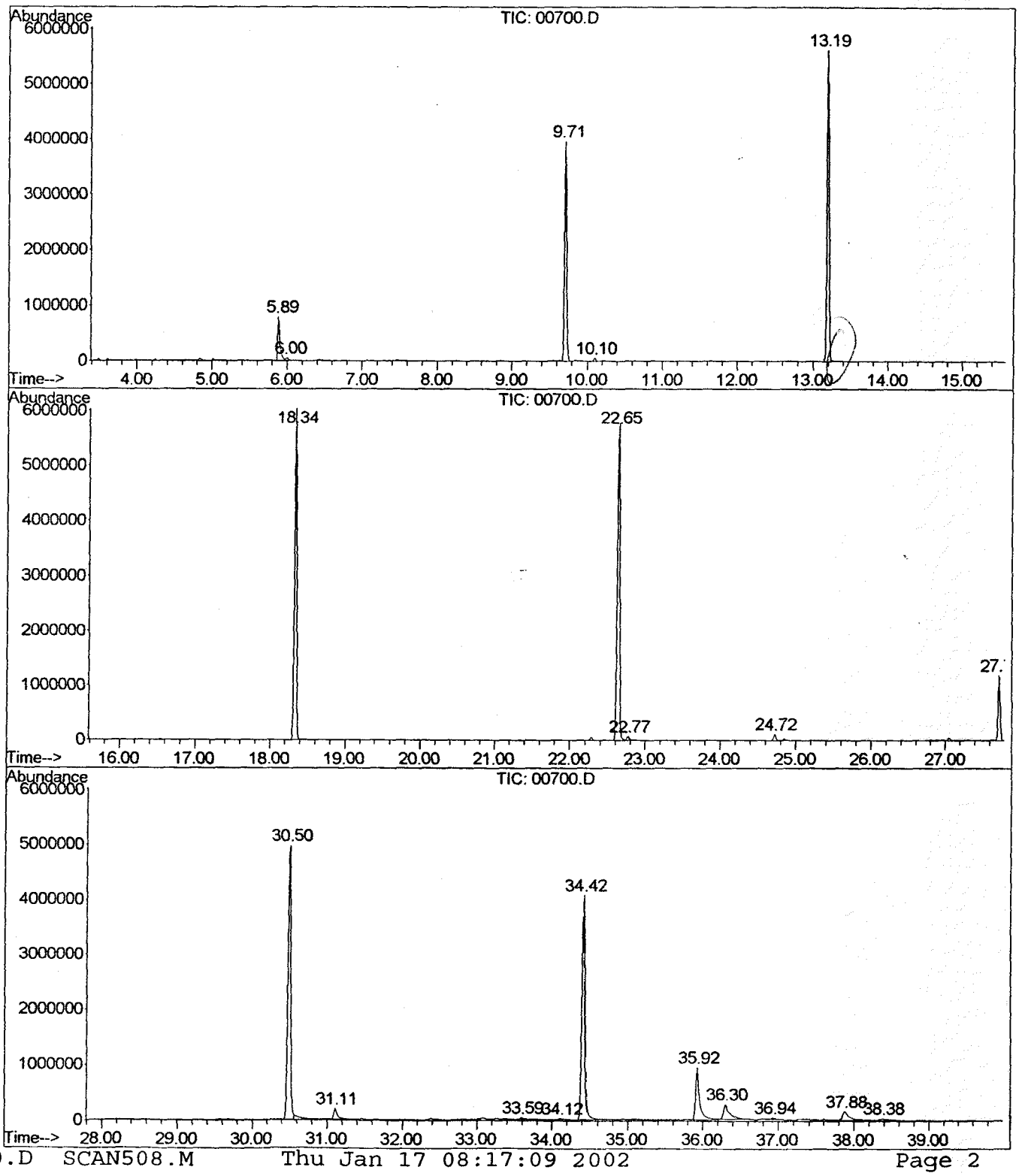
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.885	217	220	227	rBV	792694	1574665	12.05%	2.027%
2	6.000	227	230	235	rVB	52521	109749	0.84%	0.141%
3	9.710	551	555	561	rVV	3967210	7350554	56.27%	9.462%
4	10.098	585	589	593	rVV2	55533	99374	0.76%	0.128%
5	13.192	855	860	865	rBV	5622141	10646120	81.50%	13.704%
6	18.341	1305	1311	1315	rBV	6036005	11962213	91.58%	15.398%
7	22.645	1681	1688	1693	rBV	5773200	13062460	100.00%	16.815%
8	22.771	1695	1699	1703	rVB	65955	144273	1.10%	0.186%
9	24.723	1865	1870	1875	rBV2	114854	246429	1.89%	0.317%
10	27.726	2129	2133	2139	rBV	1187713	2133847	16.34%	2.747%
11	30.500	2369	2376	2381	rBV	4978175	12570204	96.23%	16.181%
12	31.105	2425	2429	2455	rVB	194459	688672	5.27%	0.886%
13	33.594	2643	2647	2659	rVB2	36017	120586	0.92%	0.155%
14	34.119	2689	2693	2707	rBV3	28517	109984	0.84%	0.142%
15	34.416	2713	2719	2749	rBV	4068446	10495550	80.35%	13.510%
16	35.923	2845	2851	2877	rBV2	940163	3527806	27.01%	4.541%
17	36.300	2877	2884	2907	rVV3	267141	1511372	11.57%	1.946%
18	36.939	2935	2940	2947	rVB8	30595	139843	1.07%	0.180%
19	37.876	3015	3022	3053	rVB4	156781	949795	7.27%	1.223%
20	38.378	3059	3066	3083	rBV4	34309	241229	1.85%	0.311%

Sum of corrected areas: 77684725

)700.D SCAN508.M Thu Jan 17 08:17:08 2002 Page 1

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN16\00700.D
Operator :
Acquired : 16 Jan 2002 2:11 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508scan
Misc Info : January 16, 2002
Vial Number: 5
Quant File :SCAN508.RES (RTE Integrator)



Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

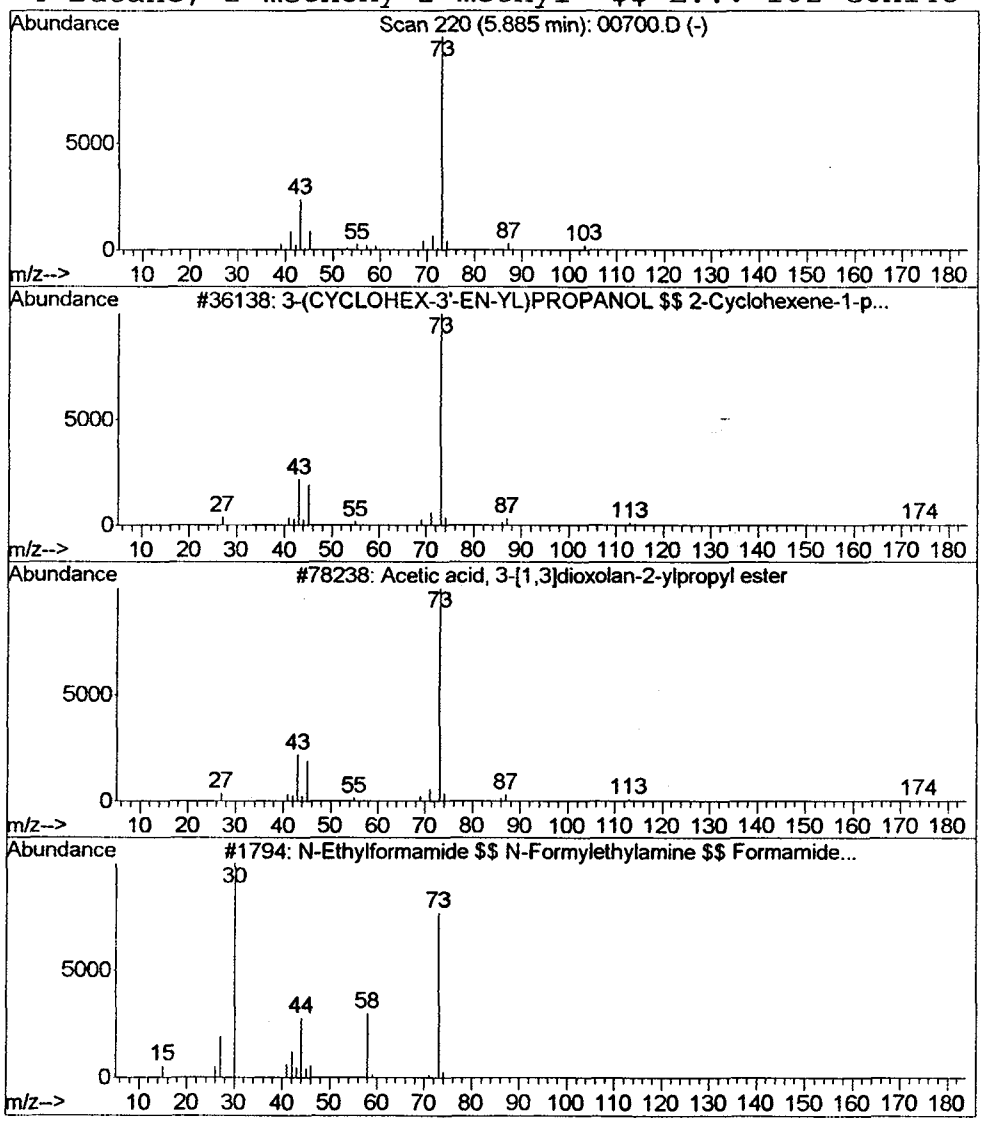
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

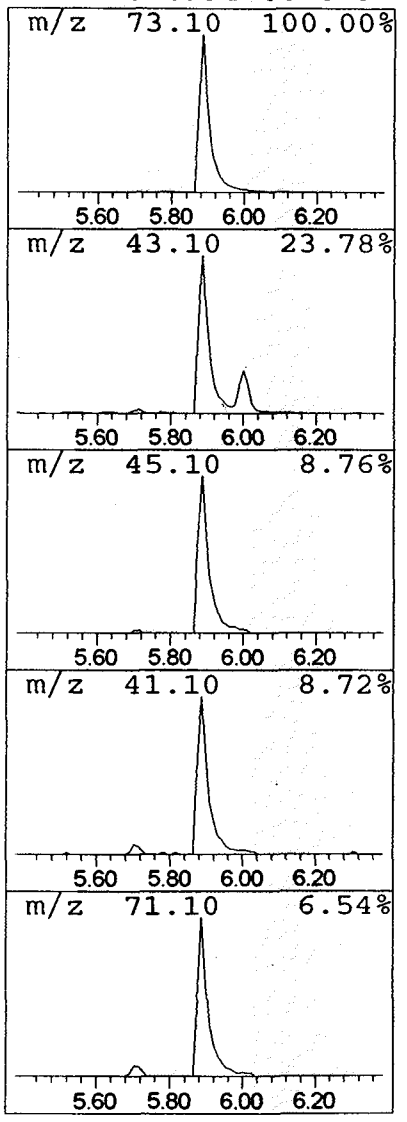
****

Peak Number 1 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.89	4.28 ug/L	1574670	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	36
2	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	36
3	N-Ethylformamide $$ N-Formylethy...	73	C3H7NO	000627-45-2	9
4	Butane, 2-methoxy-2-methyl- $$ E...	102	C6H14O	000994-05-8	9





Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

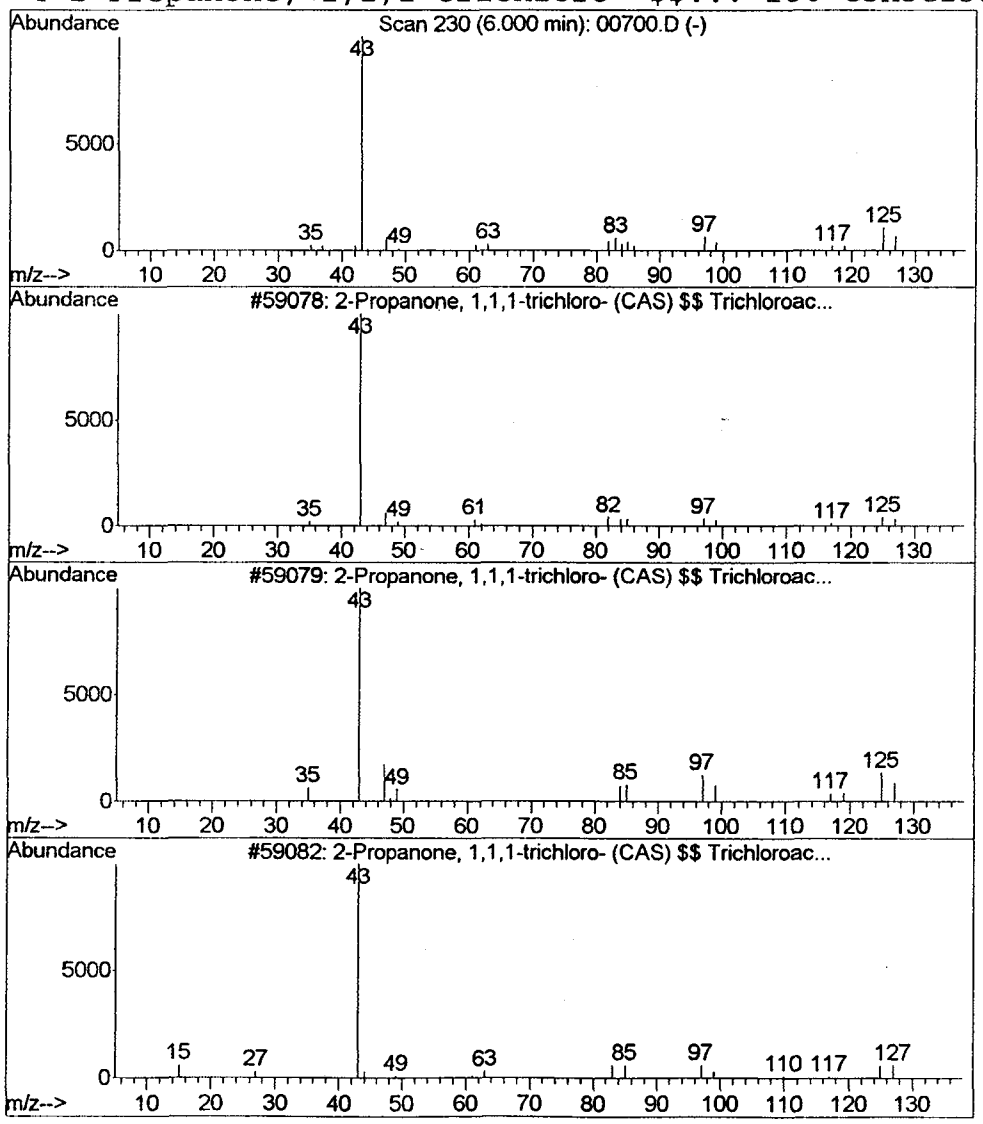
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

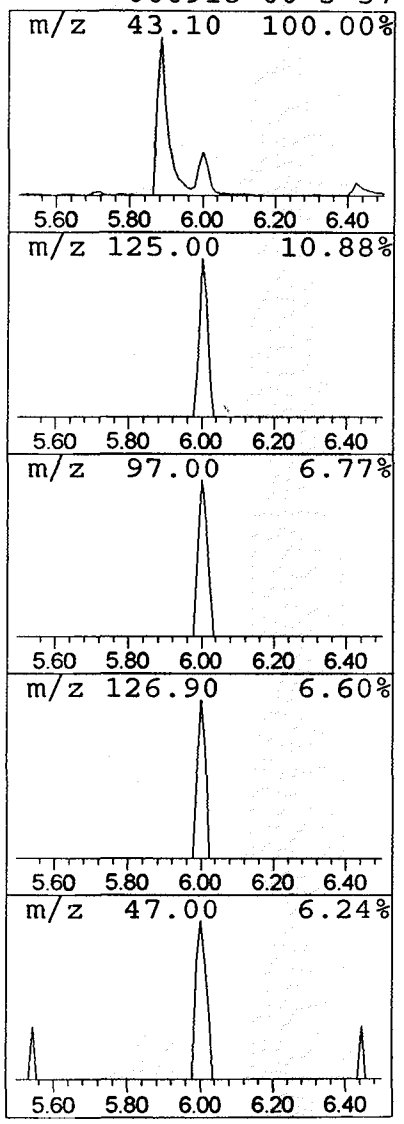
****

Peak Number 2 2-Propanone, 1,1,1-trichlor... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.00	0.30 ug/L	109749	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	59
2	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	56
3	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	53
4	2-Propanone, 1,1,1-trichloro- $$...	160	C3H3Cl3O	000918-00-3	37





Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

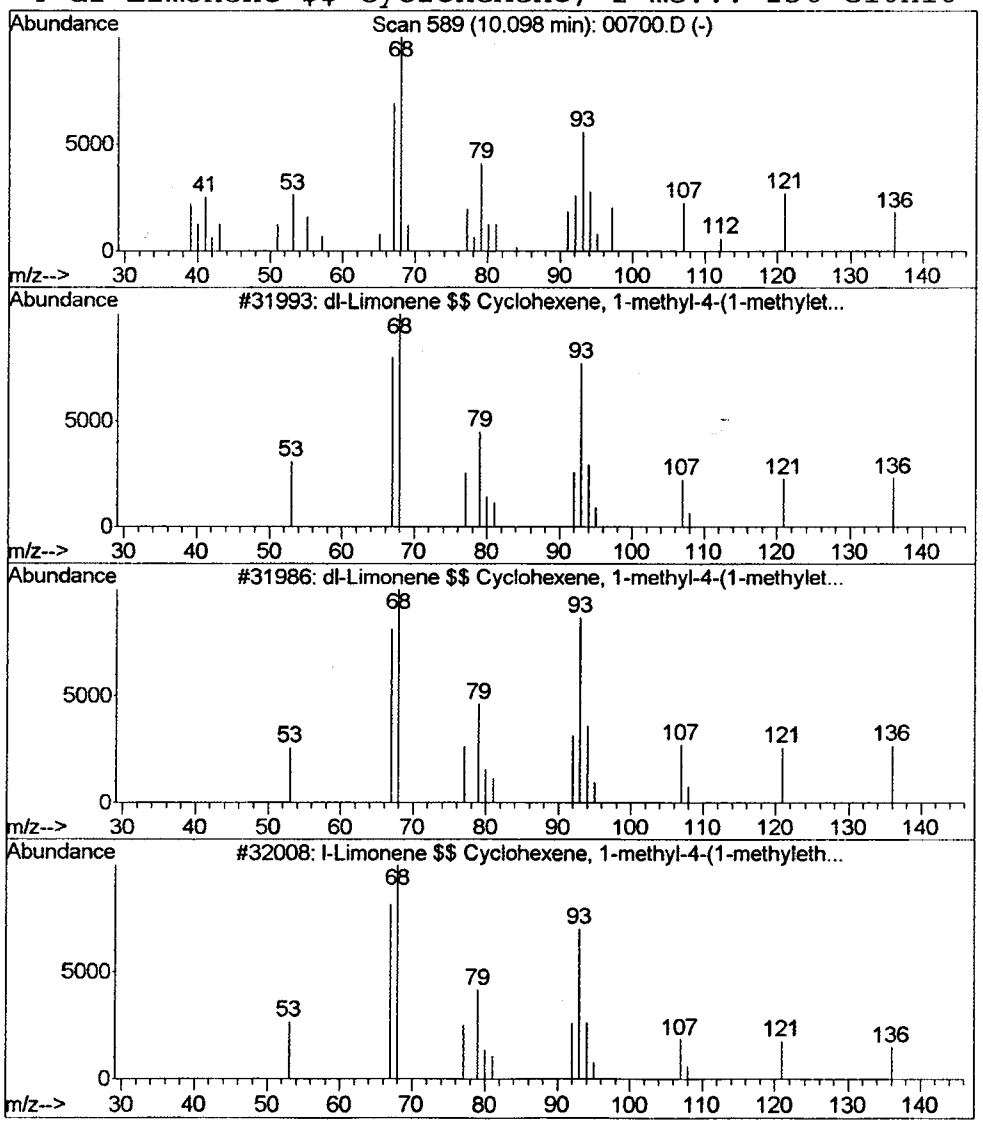
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

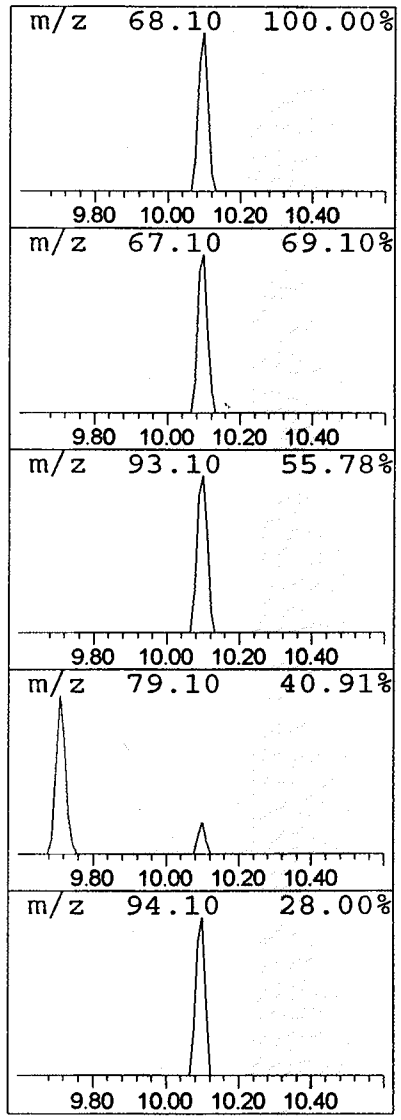
****

Peak Number 3 dl-Limonene $$ Cyclohexene,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.10	0.27 ug/L	99374	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	dl-Limonene $$ Cyclohexene, 1-me...	136	C10H16	000138-86-3	98
2	dl-Limonene $$ Cyclohexene, 1-me...	136	C10H16	000138-86-3	95
3	l-Limonene $$ Cyclohexene, 1-met...	136	C10H16	005989-54-8	95
4	dl-Limonene $$ Cyclohexene, 1-me...	136	C10H16	000138-86-3	95





Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

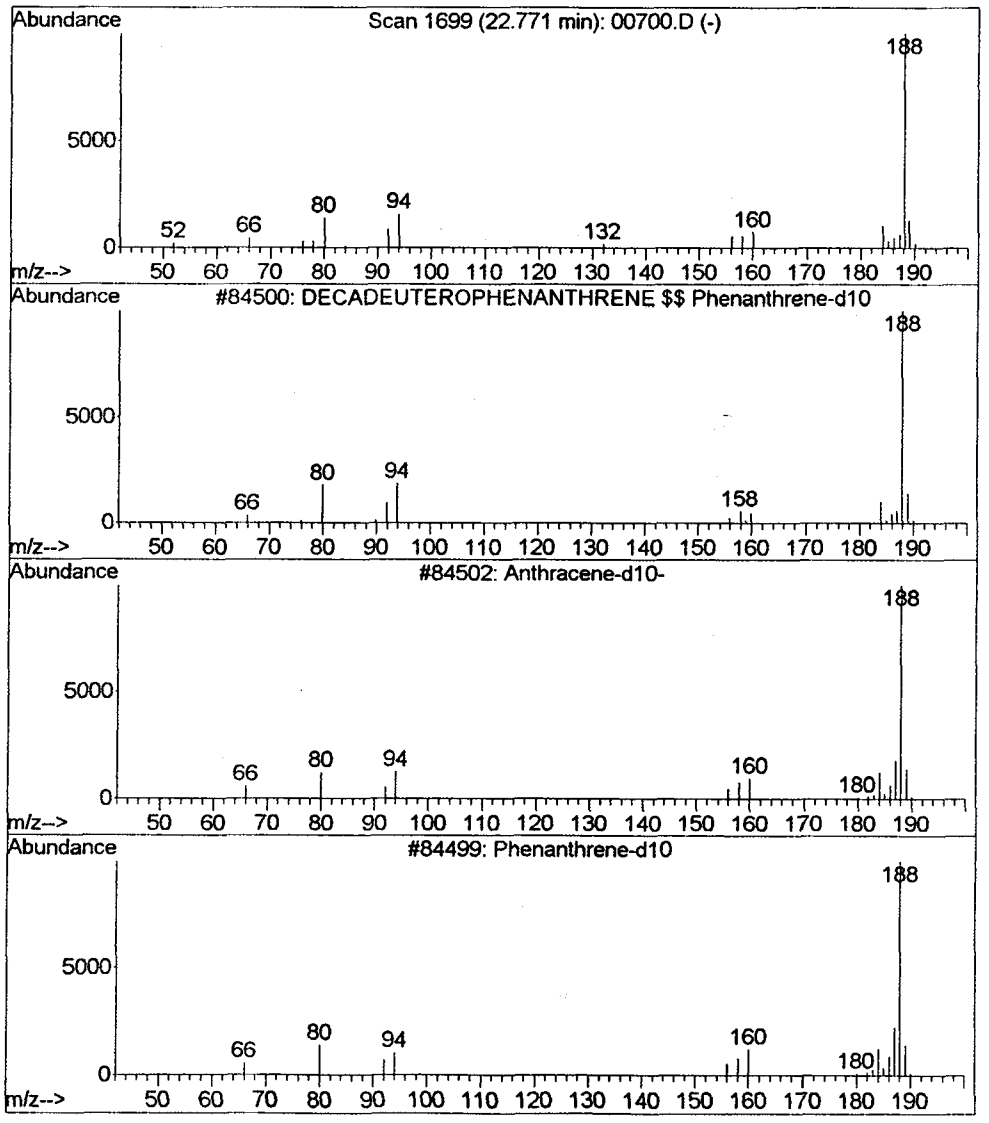
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

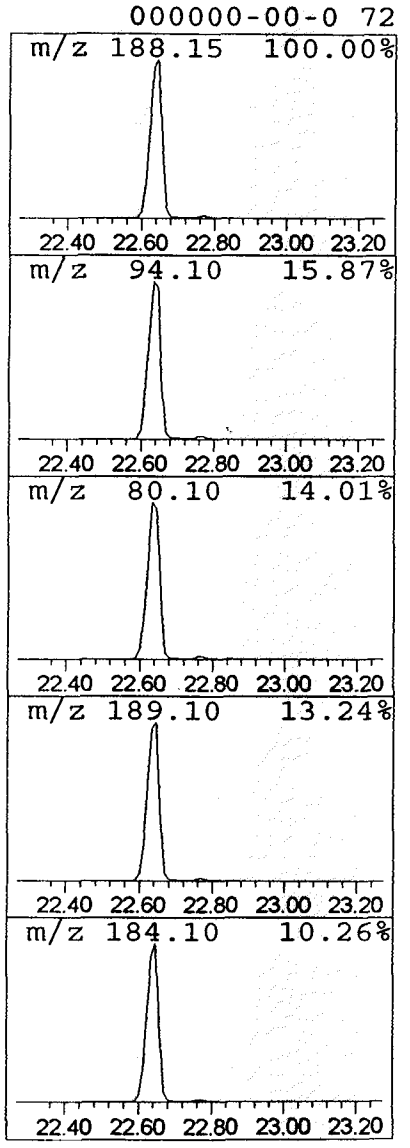
****

Peak Number 4 DECADEUTEROPHENANTHRENE $$ ... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.22 ug/L	144273	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	94
2	Anthracene-d10-	188	C14D10	001719-06-8	91
3	Phenanthrene-d10	188	C14D10	001517-22-2	80
4	Anthracene-D10	188	C14D10	000000-00-0	72





Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

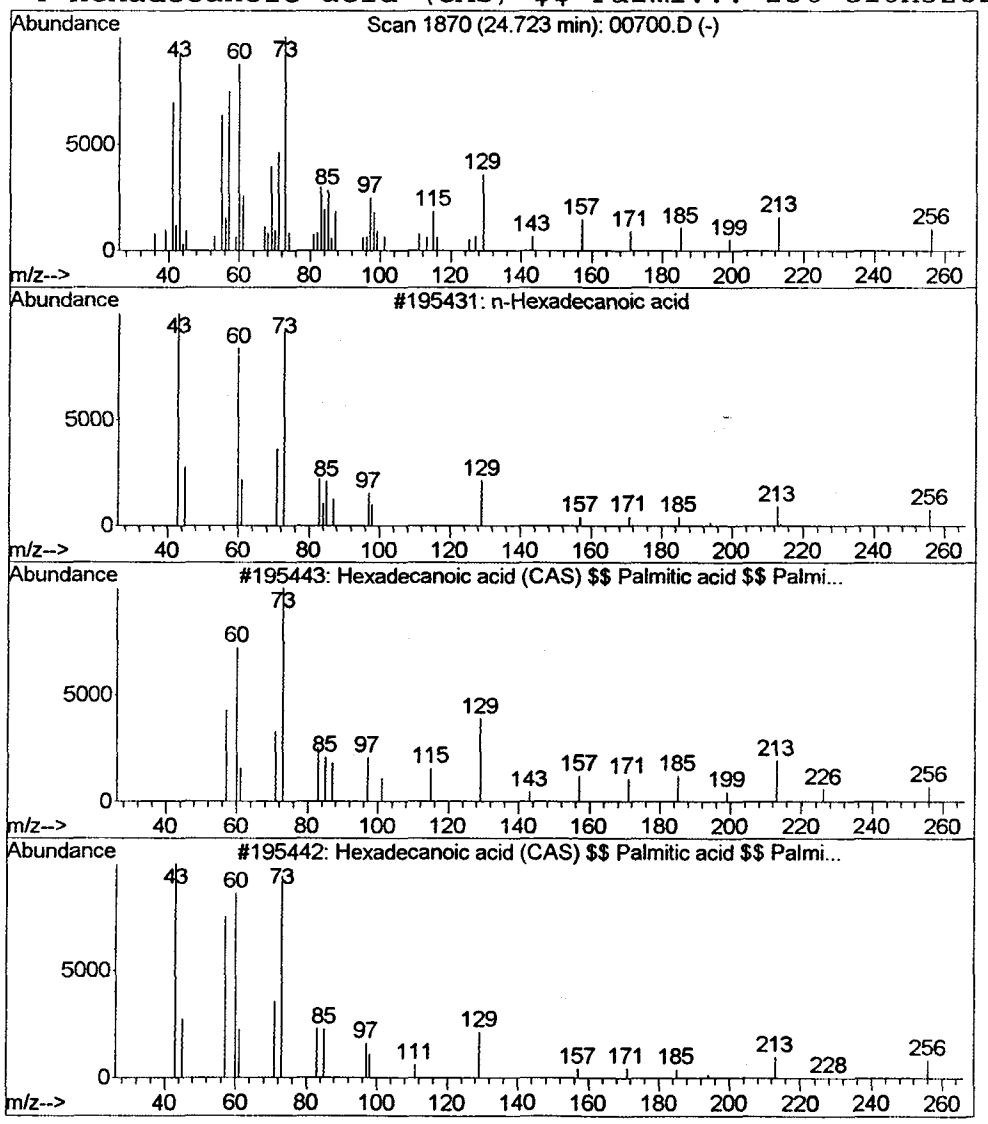
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

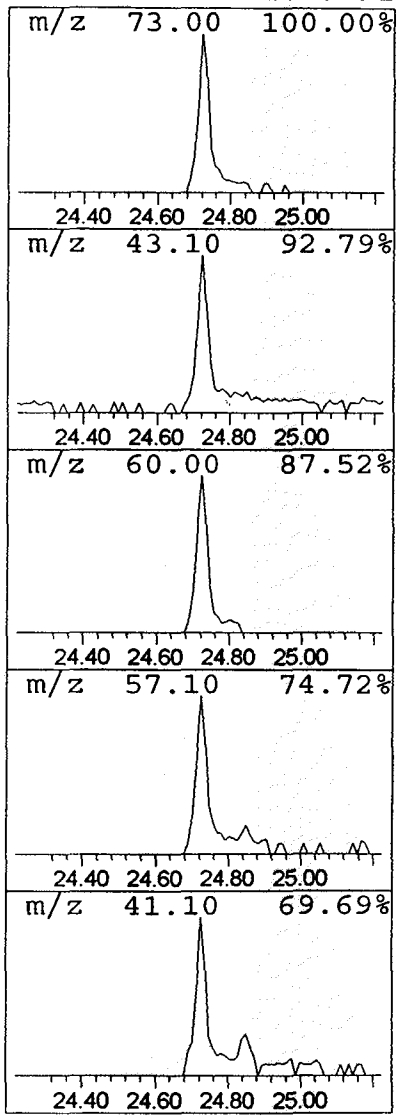
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.72	0.38 ug/L	246429	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Hexadecanoic acid (CAS) $$ Palmi...	256	C16H32O2	000057-10-3	93
3	Hexadecanoic acid (CAS) $$ Palmi...	256	C16H32O2	000057-10-3	91
4	Hexadecanoic acid (CAS) $$ Palmi...	256	C16H32O2	000057-10-3	91





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Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D          Vial: 5
Acq On    : 16 Jan 2002    2:11 pm                    Operator:
Sample    : 508scan                                   Inst    : Instrumen
Misc      : January 16, 2002                          Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title        : 508 scan method
Library      : C:\DATABASE\WILEY7N.L
```

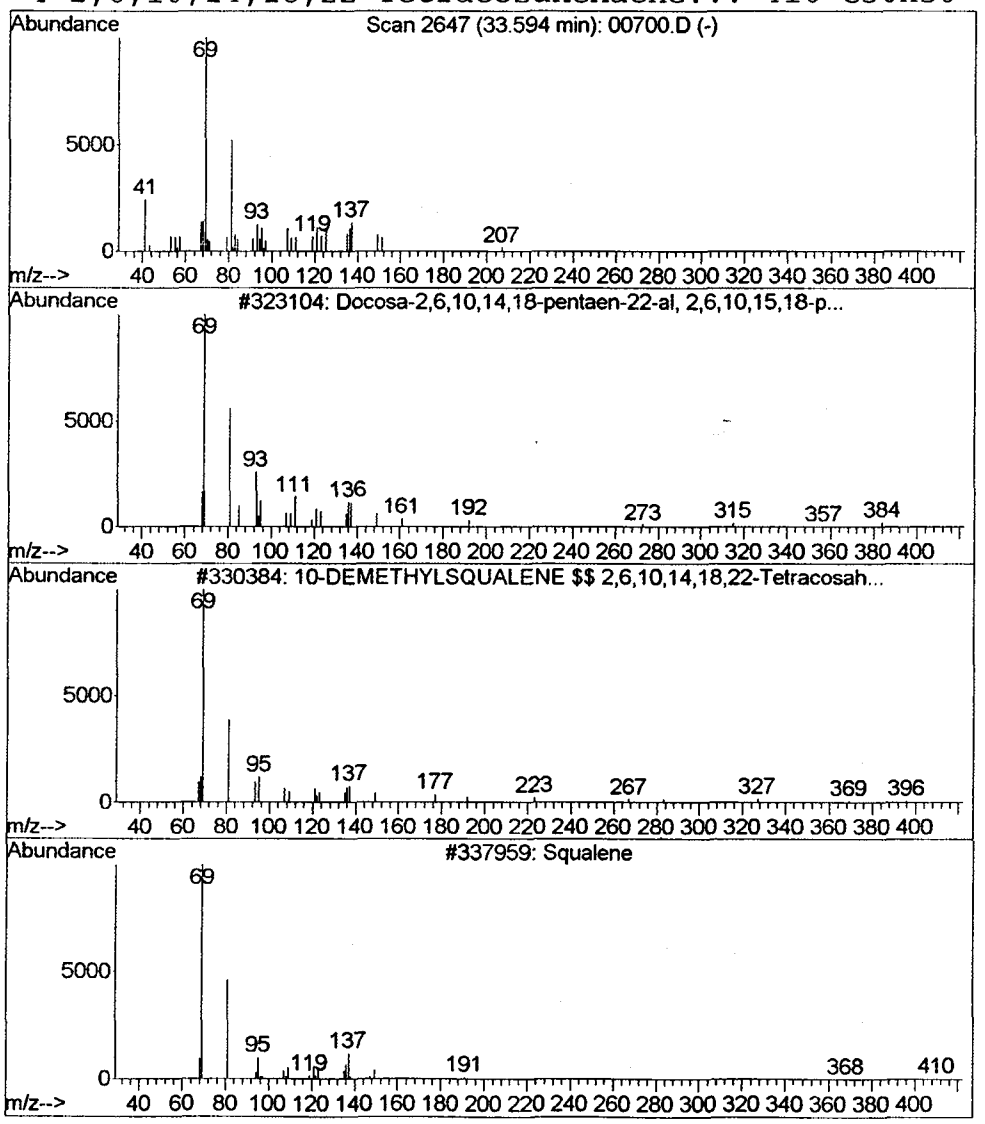
****

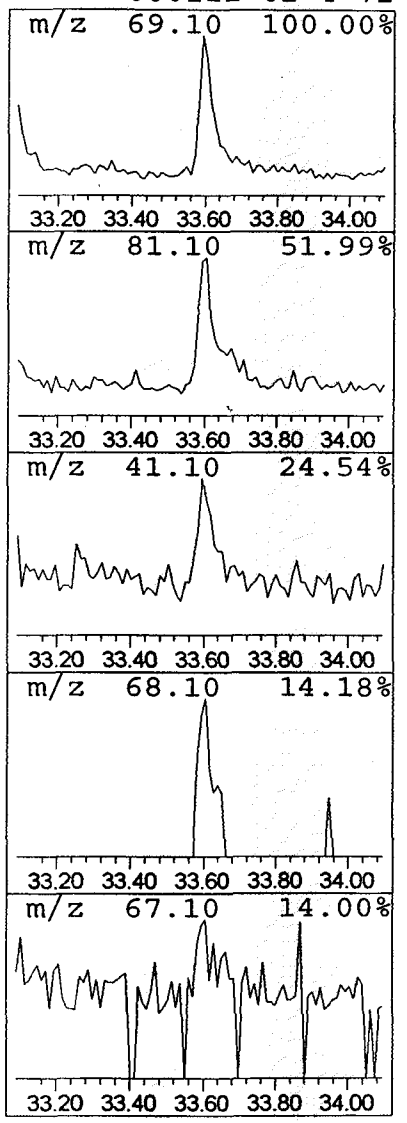
Peak Number 6 Docosa-2,6,10,14,18-pentaen... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
33.59	0.23 ug/L	120586	Perylene-d12	34.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	000000-00-0	86
2	10-DEMETHYLSQUALENE $$ 2,6,10,14...	396	C29H48	059681-06-0	86
3	Squalene	410	C30H50	007683-64-9	80
4	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72

NO GOOD MATCH





Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

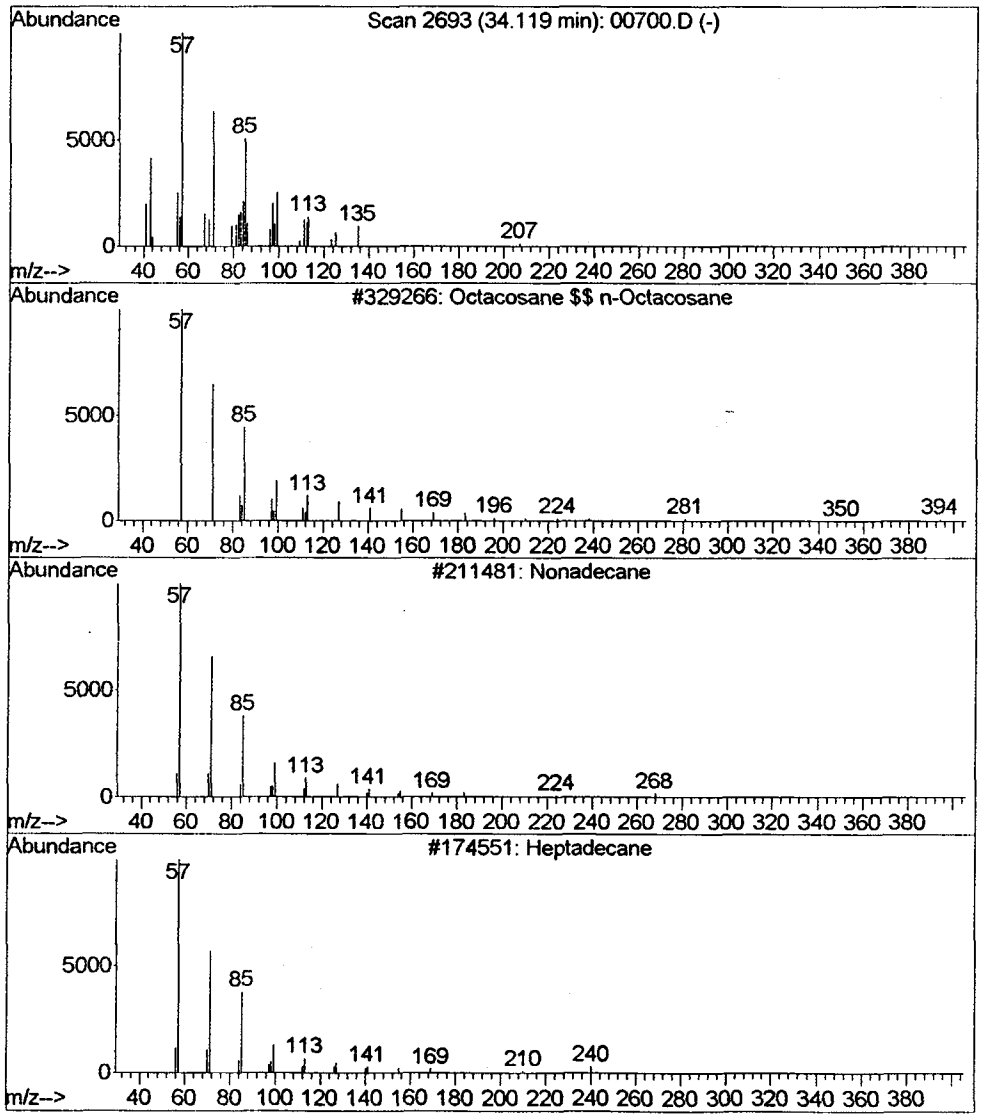
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

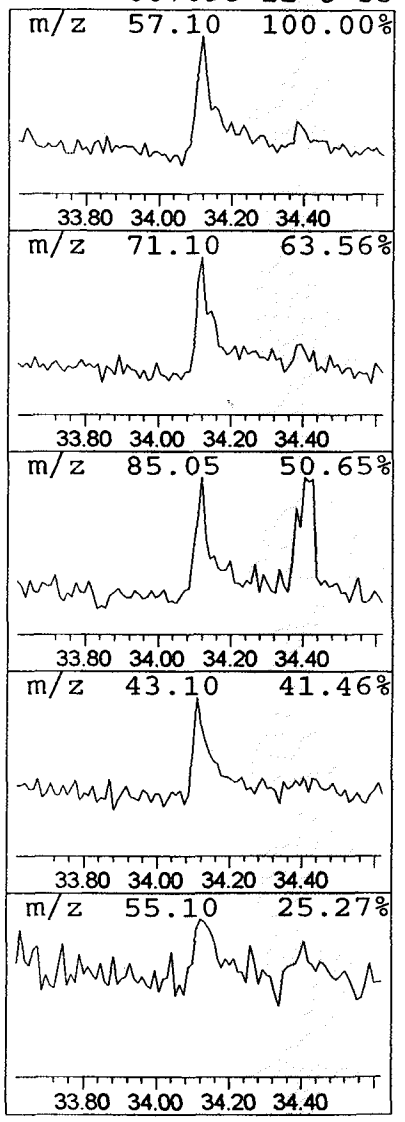
****

Peak Number 7 Octacosane $$ n-Octacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
34.12	0.21 ug/L	109984	Perylene-d12	34.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane $$ n-Octacosane	394	C28H58	000630-02-4	59
2	Nonadecane	268	C19H40	000629-92-5	53
3	Heptadecane	240	C17H36	000629-78-7	53
4	Tetratetracontane	619	C44H90	007098-22-8	53



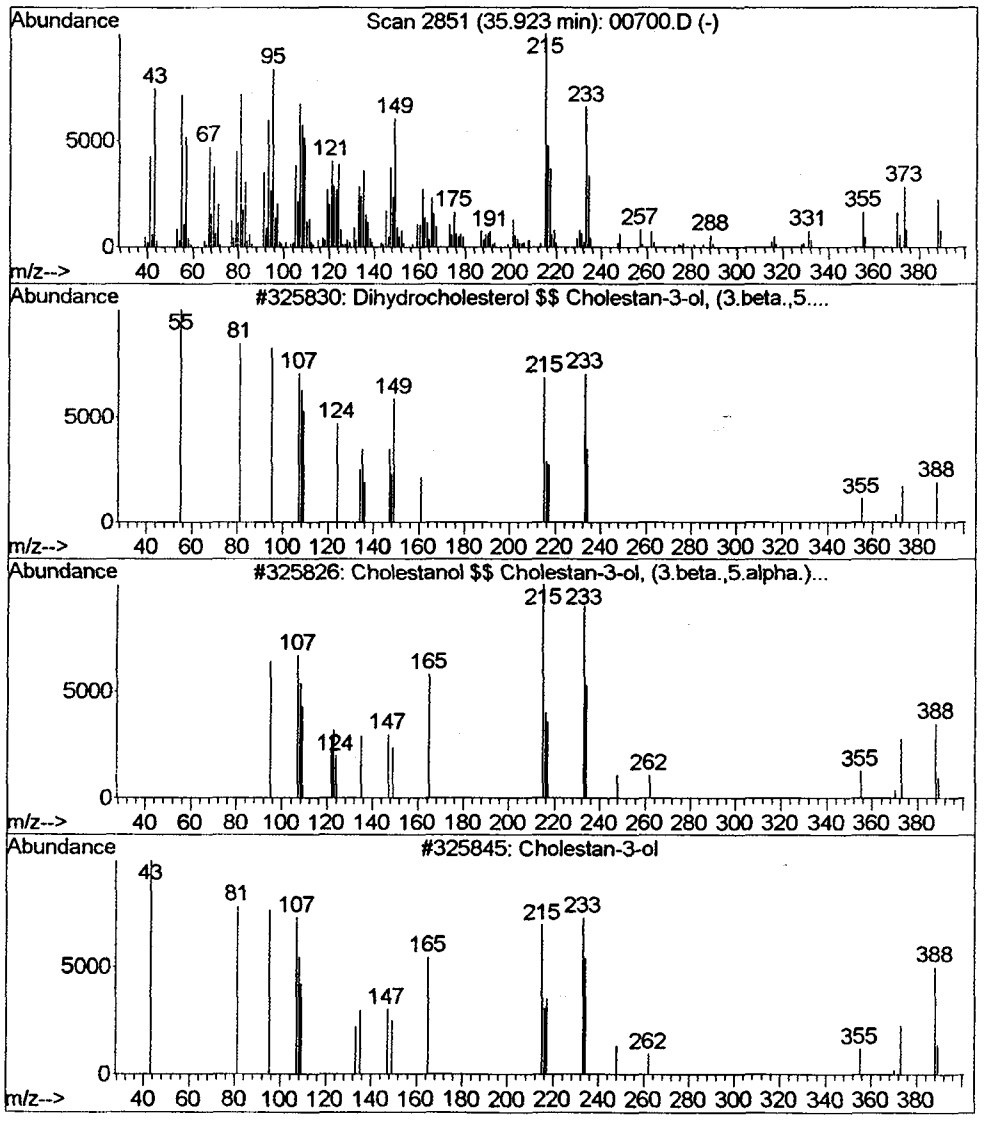


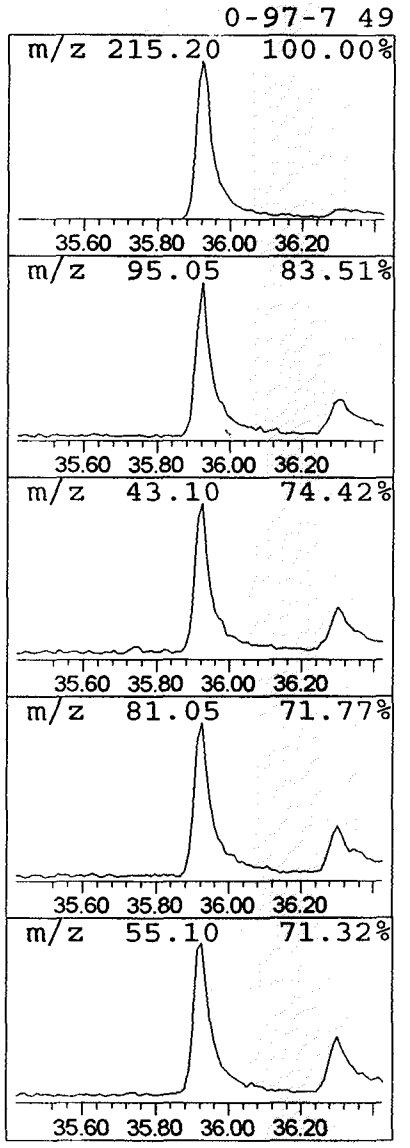
Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration

Quant Method :
Title :
Library :

possible
DIHYDROCHOLESTEROL....
although Q-value is 99, it does not appear as if the scans match very well.

Peak Number			ank 1
R.T.	EstC		R.T.
35.92	6.7		34.42
Hit# of 5			Qual
1	Dihydrocho		0-97-7 99
2	Cholestano		0-97-7 78
3	Cholestan-		9-41-2 53
4	Cholestano		0-97-7 49





Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.I

********** ***
Peak Number 9 3

Possible

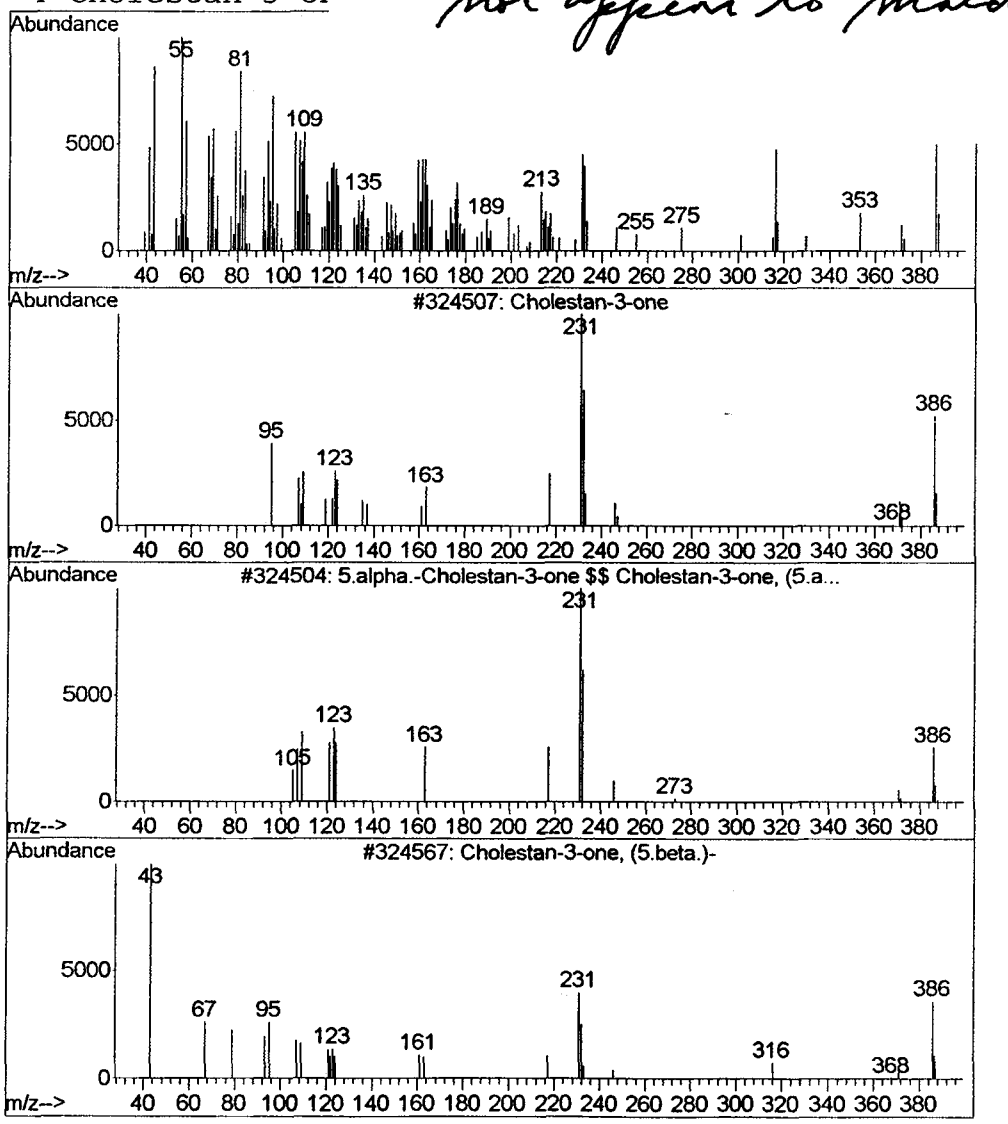
CHOLESTAN-3-ONE

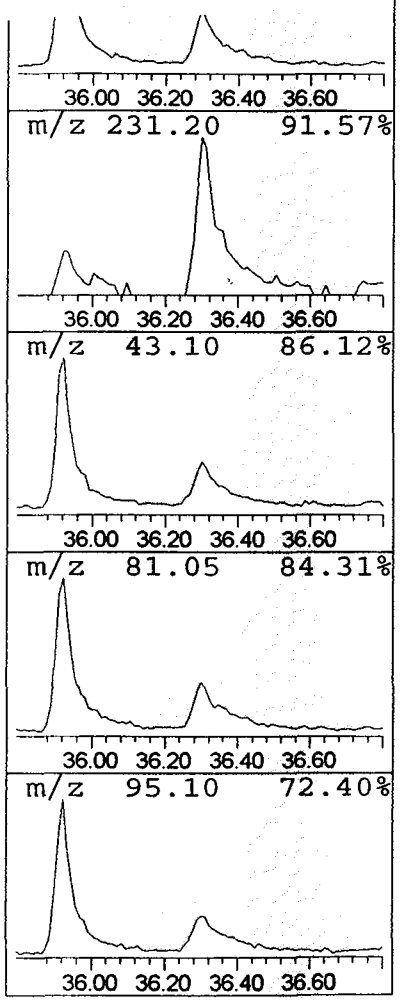
Qvalue = 95, but scans do not appears to match well.

R.T.	EstConc		
36.30	2.88 u		42

Hit# of 5	T		Qual
1	Cholestan-3-o		3-5 95
2	5.alpha.-Chole		3-1 95
3	Cholestan-3-o		3-6 89
4	Cholestan-3-o		3-5 86

)0.00%





Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

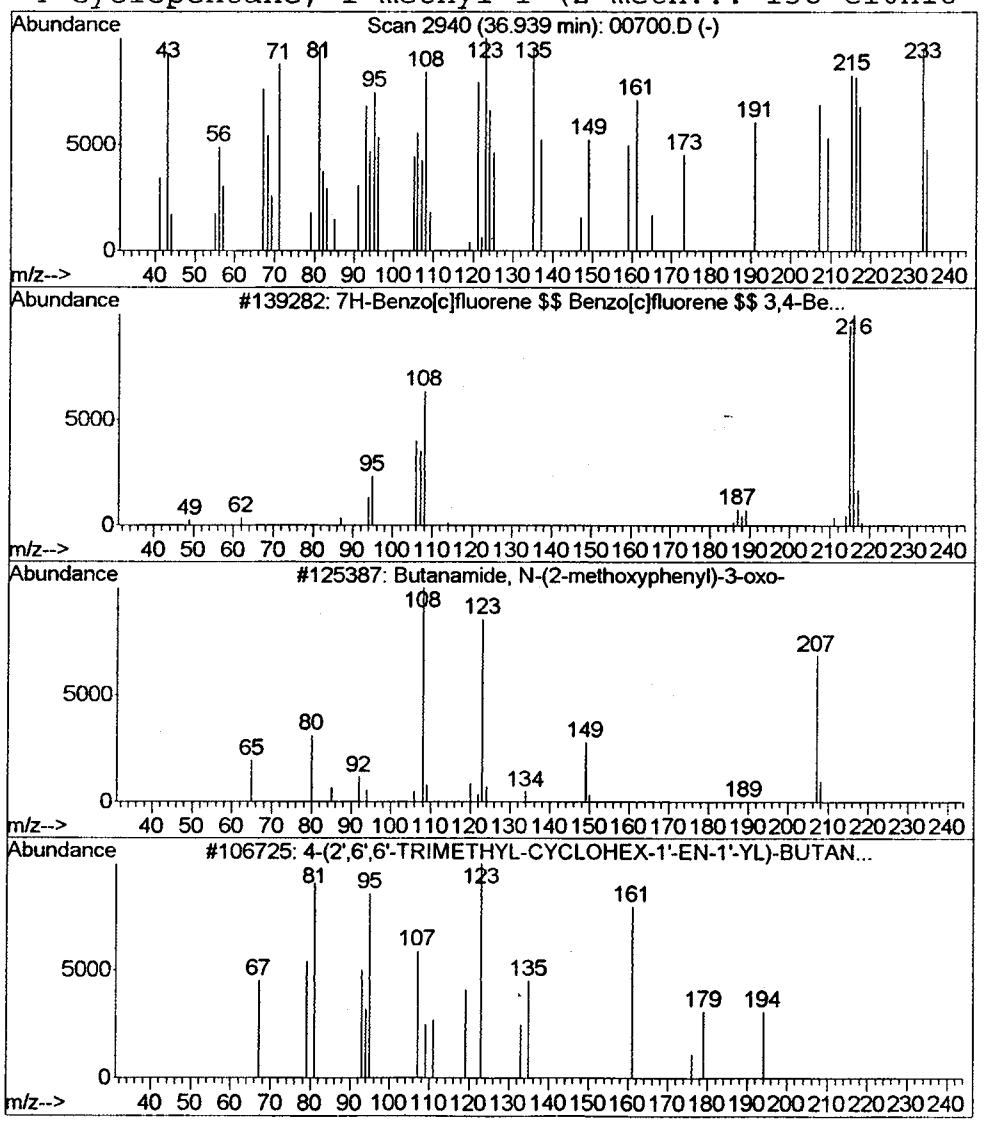
****

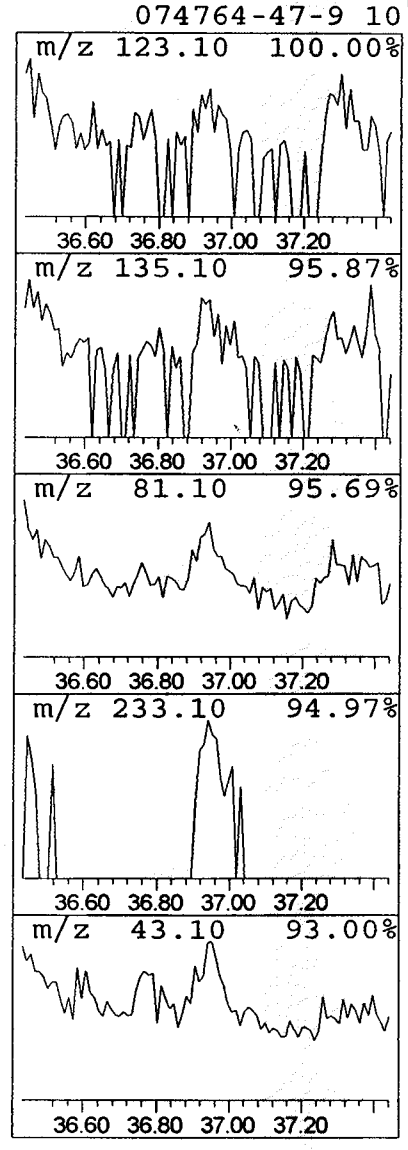
Peak Number 10 7H-Benzo[c]fluorene $$ Benz... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
36.94	0.27 ug/L	139843	Perylene-d12	34.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7H-Benzo[c]fluorene $$ Benzo[c]f...	216	C17H12	000205-12-9	27
2	Butanamide, N-(2-methoxyphenyl)-...	207	C11H13NO3	000092-15-9	10
3	4-(2',6',6'-TRIMETHYL-CYCLOHEX-1...	194	C13H22O	027758-30-1	10
4	Cyclopentane, 1-methyl-1-(2-meth...	138	C10H18	074764-47-9	10

NO GOOD MATCH





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

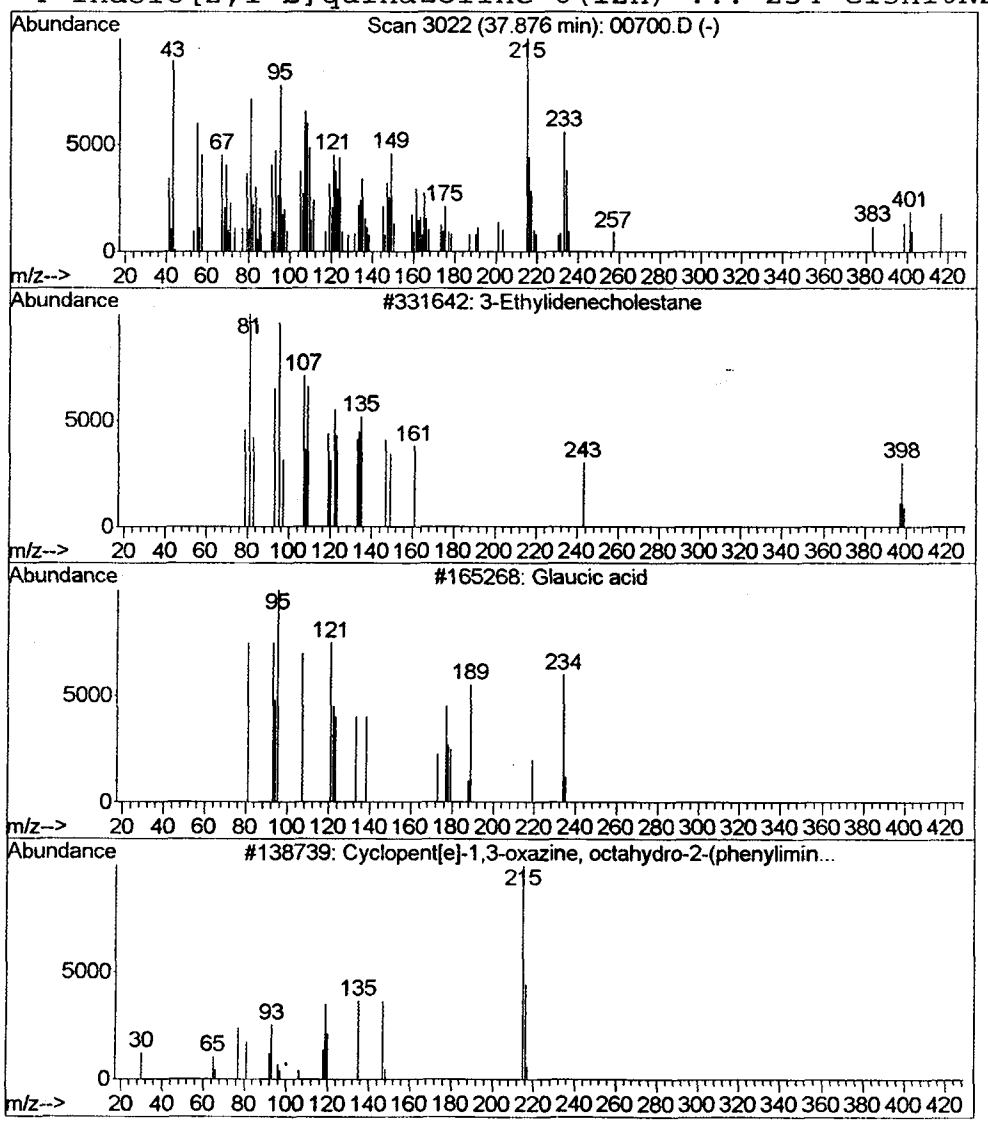
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

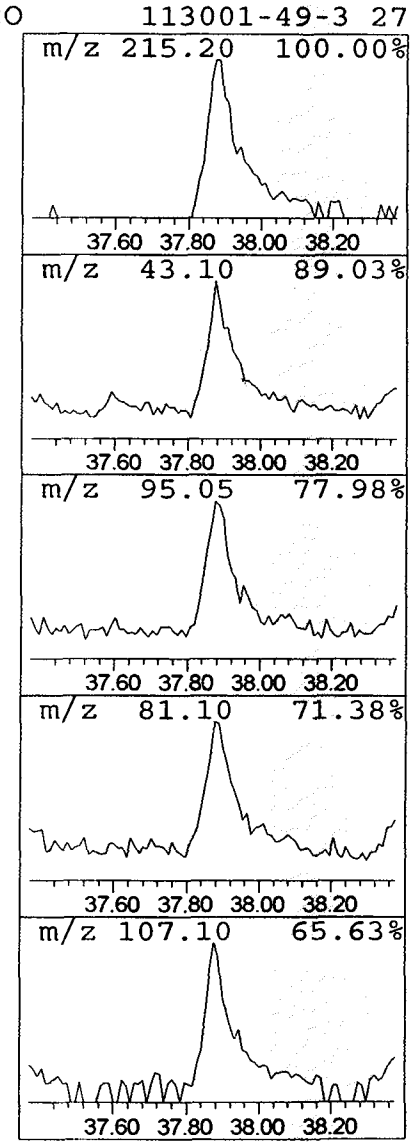
****

Peak Number 11 3-Ethylidenecholestane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
37.88	1.81 ug/L	949795	Perylene-d12	34.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Ethylidenecholestane	398	C29H50	000000-00-0	91
2	Glaucic acid	234	C15H22O2	087745-30-0	42
3	Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	000000-00-0	35
4	indolo[2,1-b]quinazoline-6(12H)-...	234	C15H10N2O	113001-49-3	27





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN16\00700.D Vial: 5
Acq On : 16 Jan 2002 2:11 pm Operator:
Sample : 508scan Inst : Instrumen
Misc : January 16, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

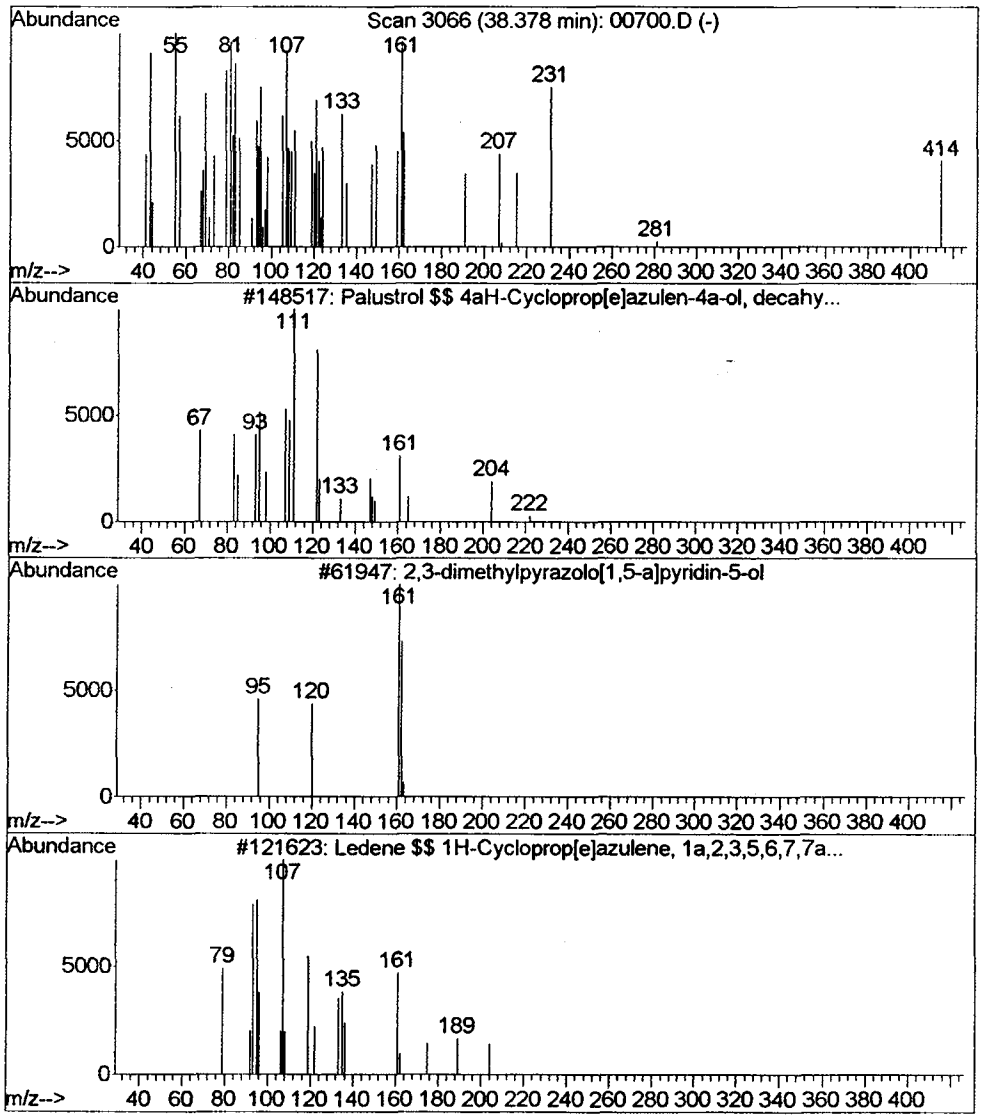
****

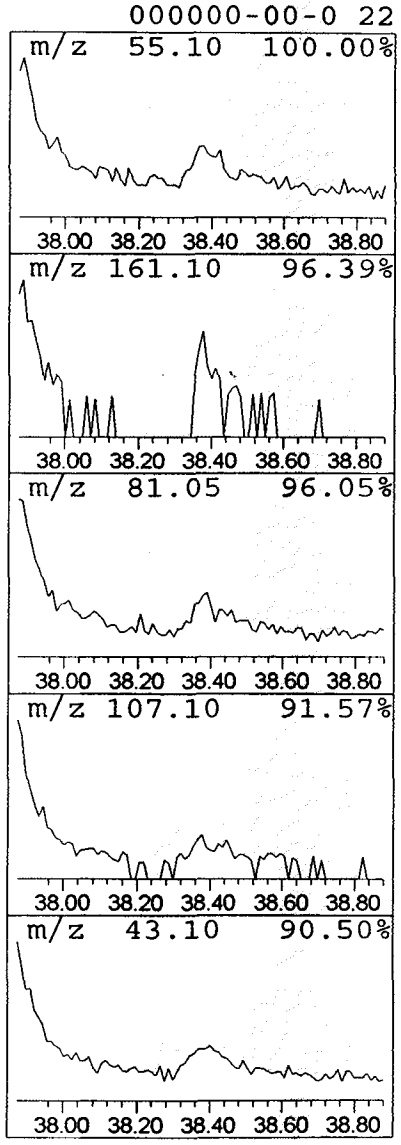
Peak Number 12 Palustrol $$ 4aH-Cycloprop[... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
38.38	0.46 ug/L	241229	Perylene-d12	34.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Palustrol $$ 4aH-Cycloprop[e]azu...	222	C15H26O	005986-49-2	25
2	2,3-dimethylpyrazolo[1,5-a]pyrid...	162	C9H10N2O	000000-00-0	22
3	Ledene $$ 1H-Cycloprop[e]azulene...	204	C15H24	021747-46-6	22
4	.beta.-Panasinsene	204	C15H24	000000-00-0	22

NO GOOD MATCH





Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 16 Jan 2002 2:11 pm
Data File: C:\MSDCHEM\1\5973N\02JAN16\00700.D
Name: 508scan
Misc: January 16, 2002
Method: C:\MSDCHEM\1\METHODS\METHODS\SCAN508.M (RTE Integrator)
Title: 508 scan method
Library Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--- #	RT	Resp	Conc
3-(CYCLOHEX-3'-EN...	5.89	4.3	ug/L	1574670	1	9.71	7350550	20.0
2-Propanone, 1,1,...	6.00	0.3	ug/L	109749	1	9.71	7350550	20.0
dl-Limonene $$ Cy...	10.10	0.3	ug/L	99374	1	9.71	7350550	20.0
DECADEUTEROPHENAN...	22.77	0.2	ug/L	144273	4	22.65	13062500	20.0
n-Hexadecanoic acid	24.72	0.4	ug/L	246429	4	22.65	13062500	20.0
Docosa-2,6,10,14,...	33.59	0.2	ug/L	120586	6	34.42	10495600	20.0
Tetracosane $$ n-O...	34.12	0.2	ug/L	109984	6	34.42	10495600	20.0
Dihydrocholestero...	35.92	6.7	ug/L	3527810	6	34.42	10495600	20.0
Cholestan-3-one	36.30	2.9	ug/L	1511370	6	34.42	10495600	20.0
7H-Benzo[c]fluore...	36.94	0.3	ug/L	139843	6	34.42	10495600	20.0
3-Ethylidenechole...	37.88	1.8	ug/L	949795	6	34.42	10495600	20.0
Palustrol $$ 4aH-...	38.38	0.5	ug/L	241229	6	34.42	10495600	20.0