Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 01 08:46:01 2002 Quant Results File: SCAN508.RES

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

Organic will be reset

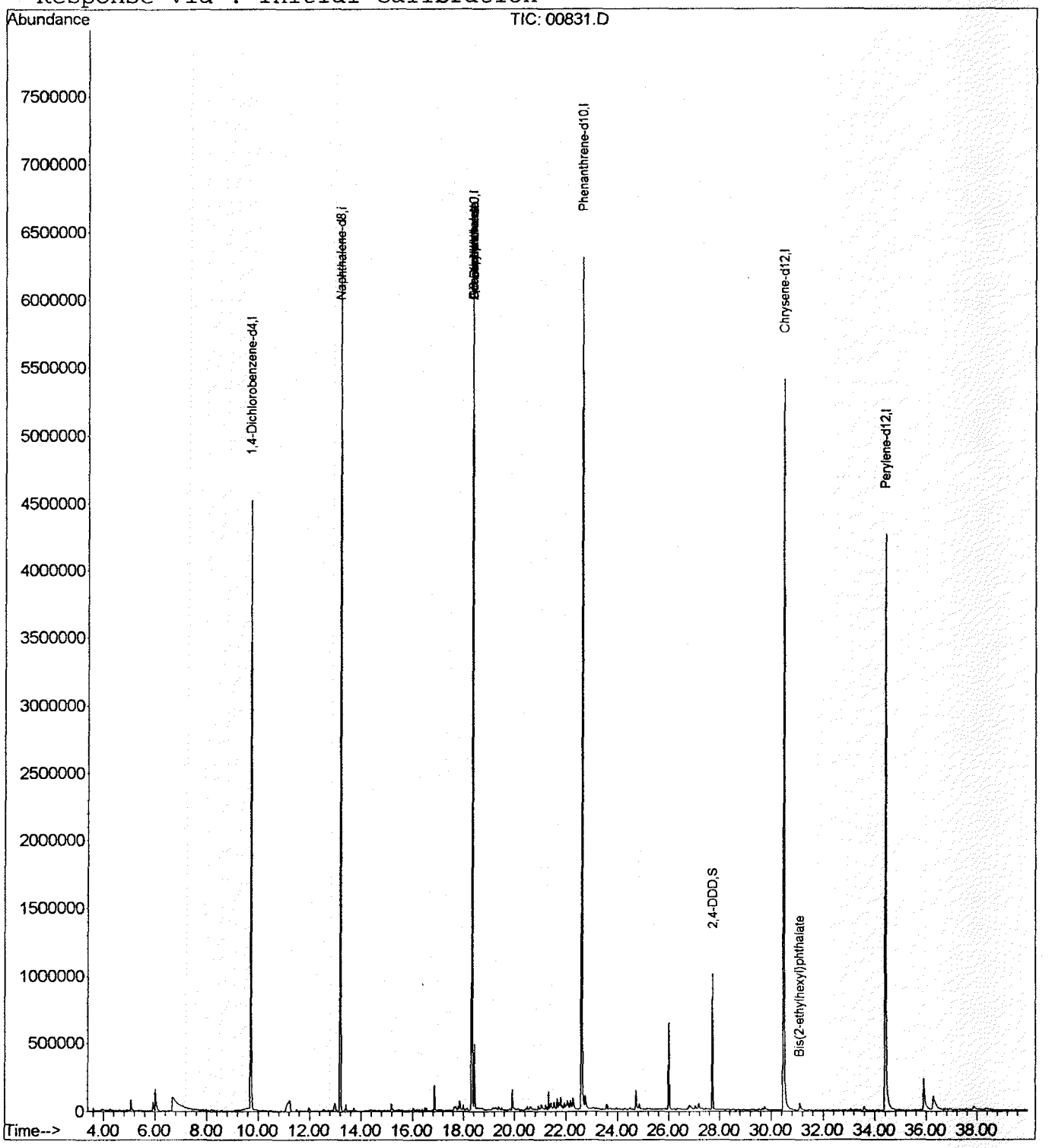
Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.71	152	1513969	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	6389561	20.00	ug/L	-0.02
17) Acenaphthene-d10	18.34	164	3350546	20.00	ug/L	-0.01
29) Phenanthrene-d10	22.65	188	5363324	20.00	ug/L	-0.02
38) Chrysene-d12	30.49	240	4706327	20.00	ug/L	-0.02
44) Perylene-d12	34.42	264	3342876	20.00	ug/L	0.00
System Monitoring Compounds						
37) 2,4-DDD	27.73	235	374711	4.42	ug/L	0.00
Spiked Amount 5.000			Recovery =	88.40%		
Target Compounds						Qvalue
20) Dimethylphthalate	18.34	163	532685	2.41	ug/L #	56
21) 2,6-Dinitrotoluene	18.34	165	421686	9.77	ug/L #	17
42) Bis(2-ethylhexyl)phthalate	31.11	149	68525	0.84	ug/L	91

(#) = qualifier out of range (m) = manual integration
00831.D SCAN508.M Fri Feb 01 15:31:30 2002 Page 1

Quantitation Report (Not Reviewed)

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 1 8:46 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\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 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

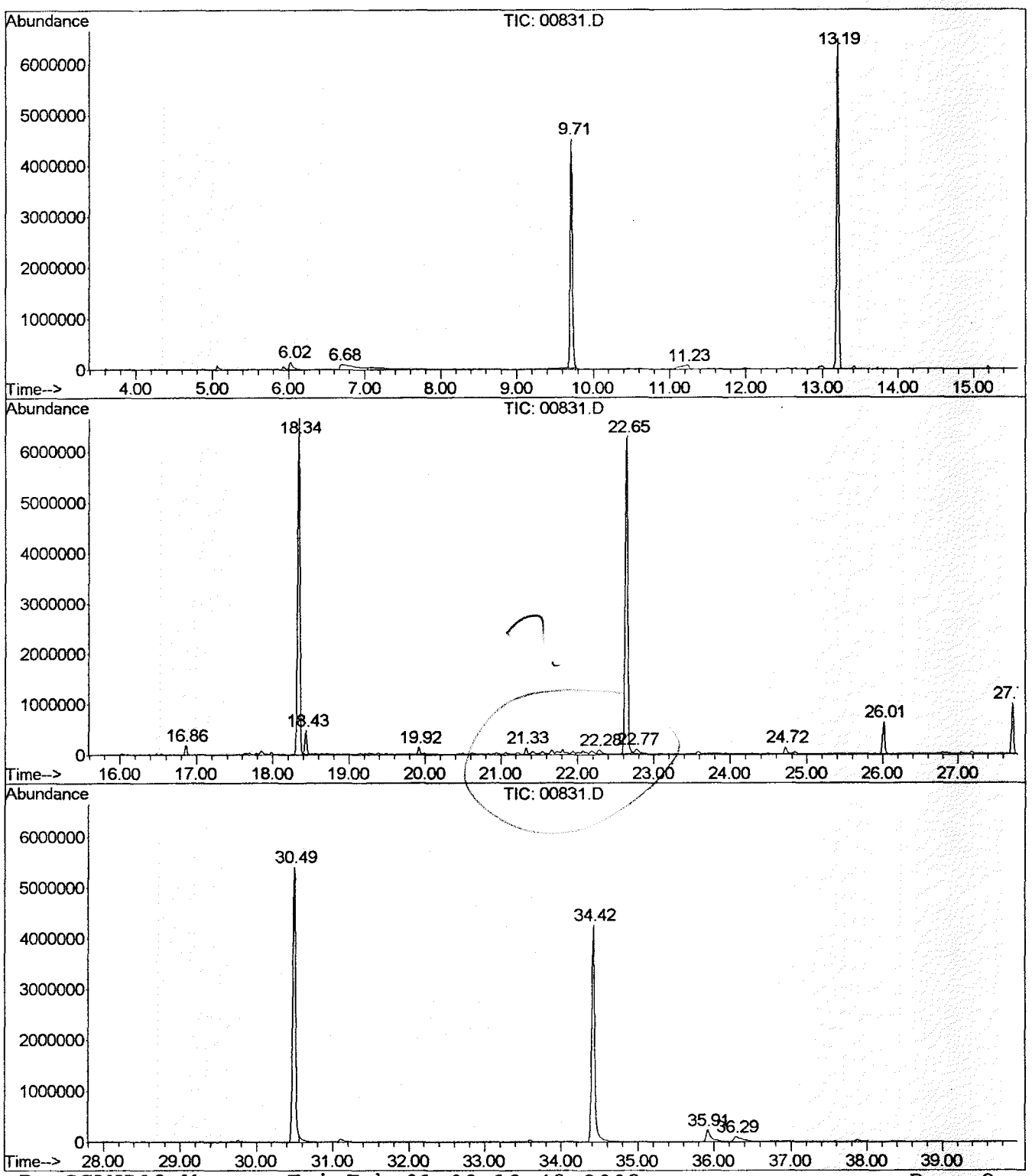
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	6.023	229	232	257	rVB	160861	515800	3.56%	0.609%
2	6.685	287	290	321	rBV3	100936	1457282	10.06%	1.720%
3	9.710	551	555	561	rBV	4496577	8730675	60.29%	10.306%
4	11.229	671	688	699	rVB3	78219	666622	4.60%	0.787%
5	13.192	855	860	865	rBV	6481207	12404241	85.66%	14.642%
6	16.857	1177	1181	1185	rBV	189953	349764	2.42%	0.413%
7	18.341	1305	1311	1315	rBV	6649282	13502969	93.25%	15.939%
8	18.433	1315	1319	1325	rVV	473837	835359	5.77%	0.986%
9	19.917	1445	1449	1453	rBV	151745	278644	1.92%	0.329%
10	21.333	1567	1573	1577	rBV	132508	251890	1.74%	0.297%
11	22.280	1653	1656	1669	rVB3	86170	297073	2.05%	0.351%
12	22.646	1681	1688	1693	rBV	6293554	14480216	100.00%	17.093%
13	22.771	1695	1699	1711	rVB3	95133	339091	2.34%	0.400%
14	24.723	1865	1870	1877	rBV	140145	322072	2.22%	0.380%
15	26.014	1977	1983	1989	rBV	632820	1260704	8.71%	1.488%
16	27.726	2127	2133	2137	rBV	997591	1853154	12.80%	2.187%
17	30.489	2369	2375	2381	rBV2	5403377	13892019	95.94%	16.398%
18	34.416	2713	2719	2751	rBV	4257600	11563258	79.86%	13.649%
19	35.912	2845	2850	2875	rBV2	225108	1011275	6.98%	1.194%
20	36.289	2875	2883	2901	rBV2	99858	703734	4.86%	0.831%

Sum of corrected areas: 84715842

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\5973N\02JAN31\00831.D
Operator :
Acquired : 31 Jan 2002 1:01 pm using AcqMethod SCAN508
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : January 31, 2002
Vial Number: 4
Quant File :SCAN508.RES (RTE Integrator)



00831.D SCAN508.M Fri Feb 01 09:18:42 2002 Page 2

Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

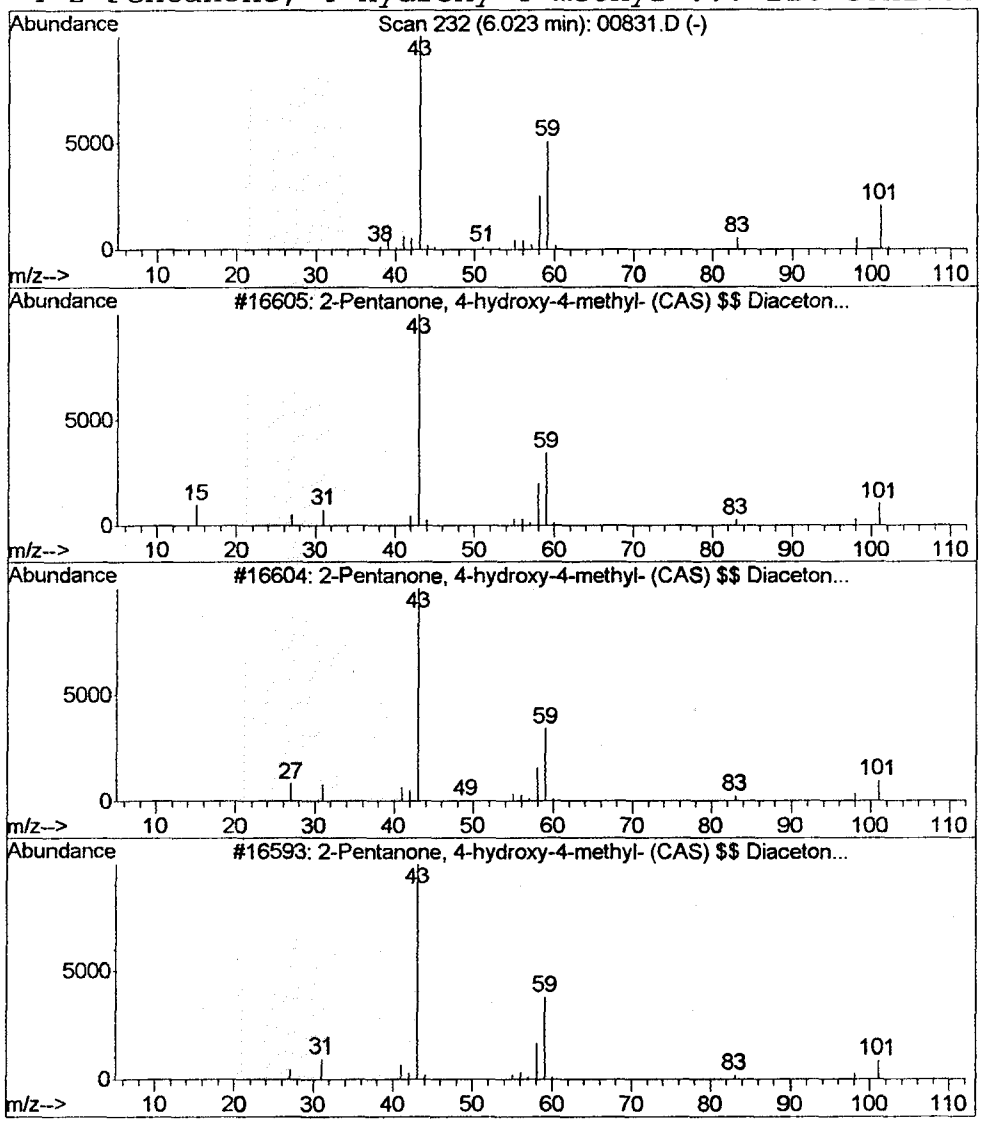
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

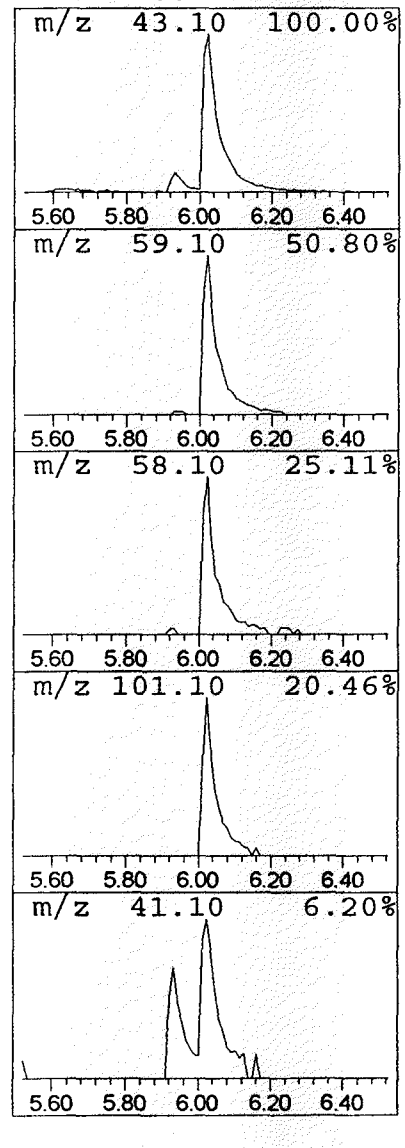
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.02	1.18 ug/L	515800	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	83
2	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	83
3	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	83
4	2-Pentanone, 4-hydroxy-4-methyl-...	116	C6H12O2	000123-42-2	78





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

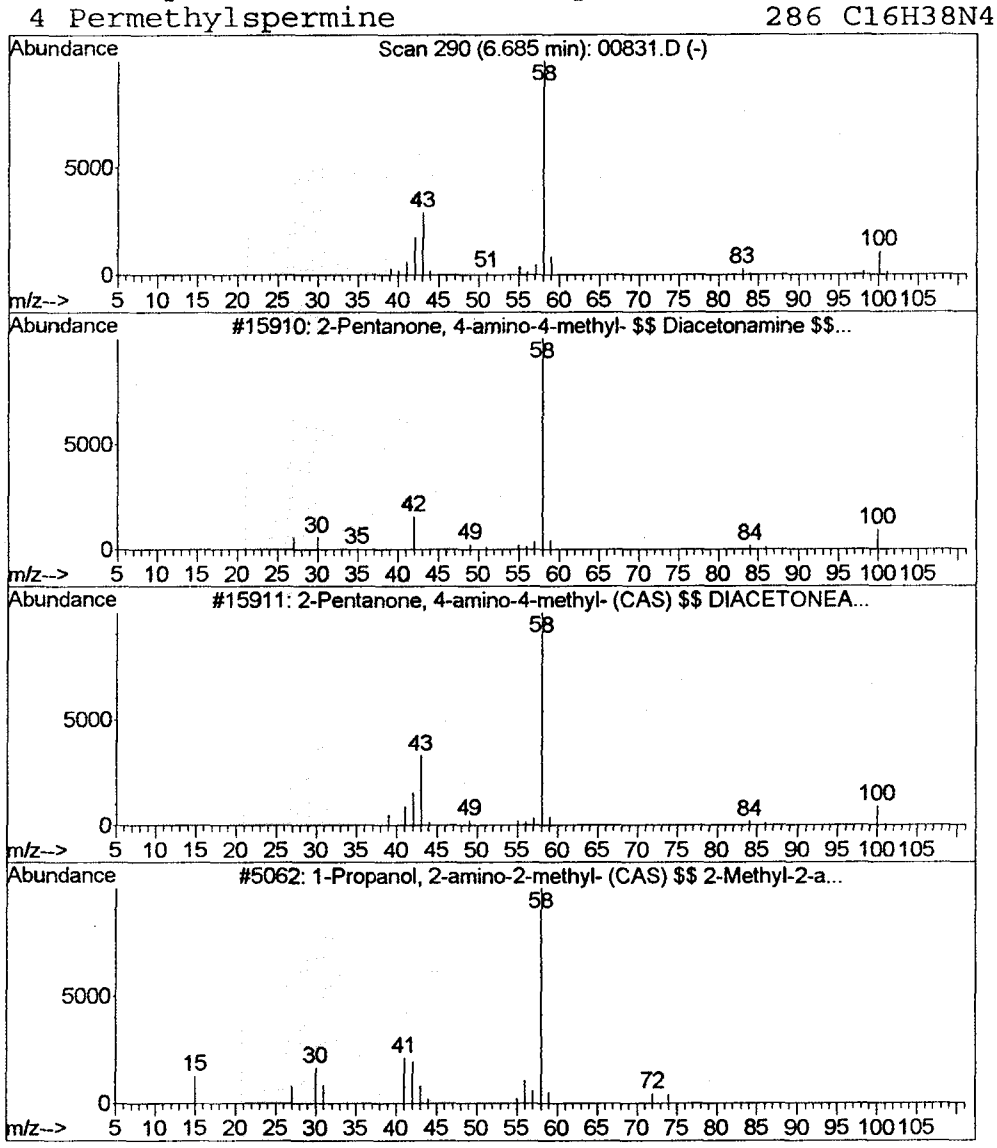
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

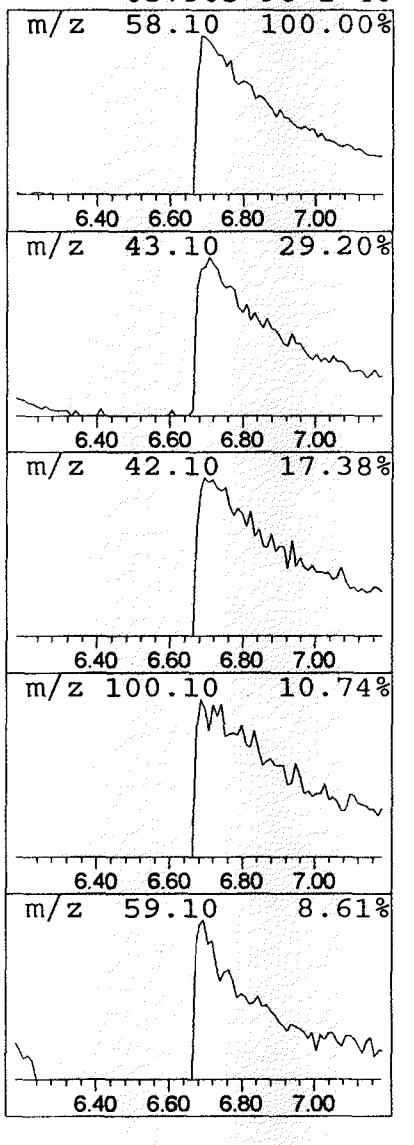
****

Peak Number 2 2-Pentanone, 4-amino-4-meth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	3.34 ug/L	1457280	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-amino-4-methyl- $...	115	C6H13NO	000625-04-7	78
2	2-Pentanone, 4-amino-4-methyl- (...	115	C6H13NO	000625-04-7	64
3	1-Propanol, 2-amino-2-methyl- (C...	89	C4H11NO	000124-68-5	50
4	Permethylspermine	286	C16H38N4	057905-96-1	40





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

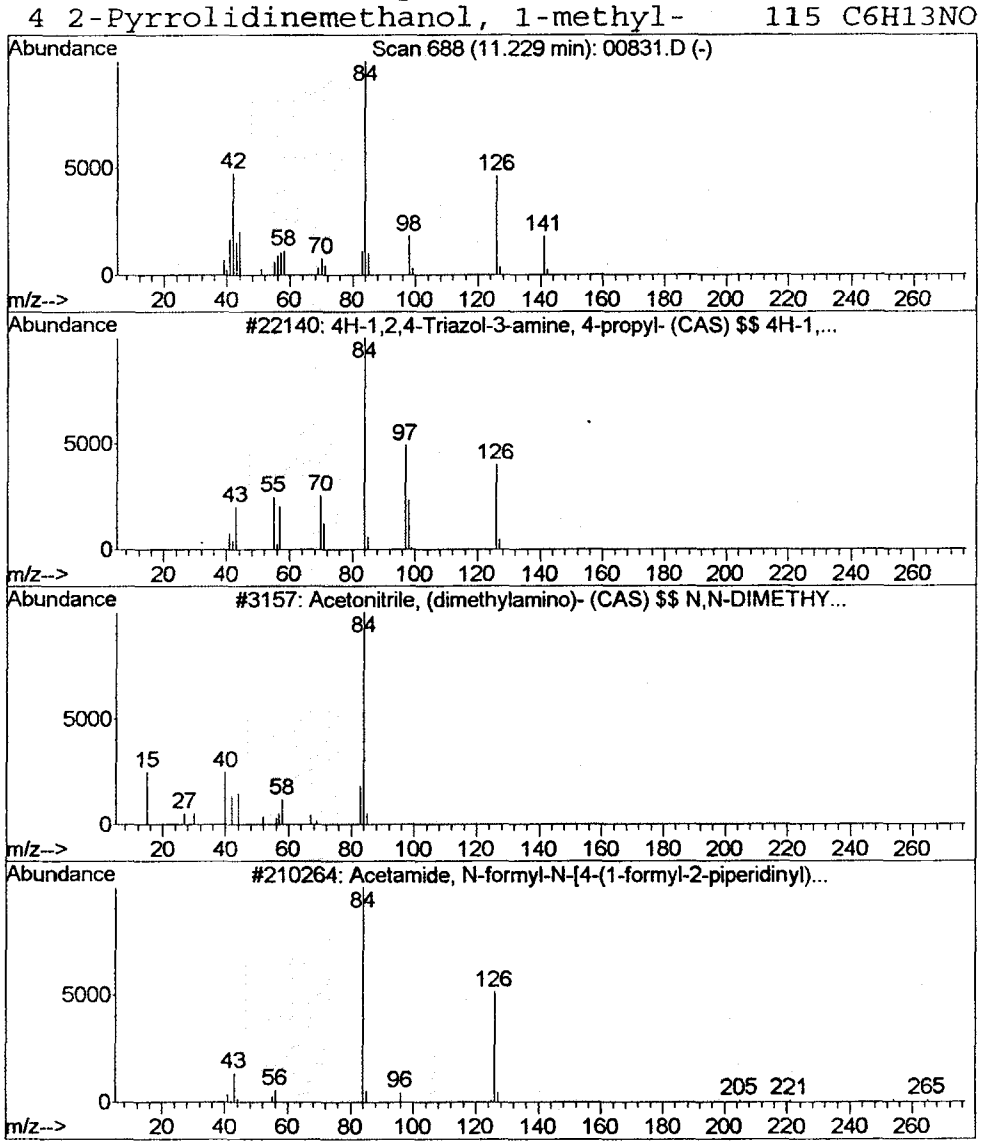
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

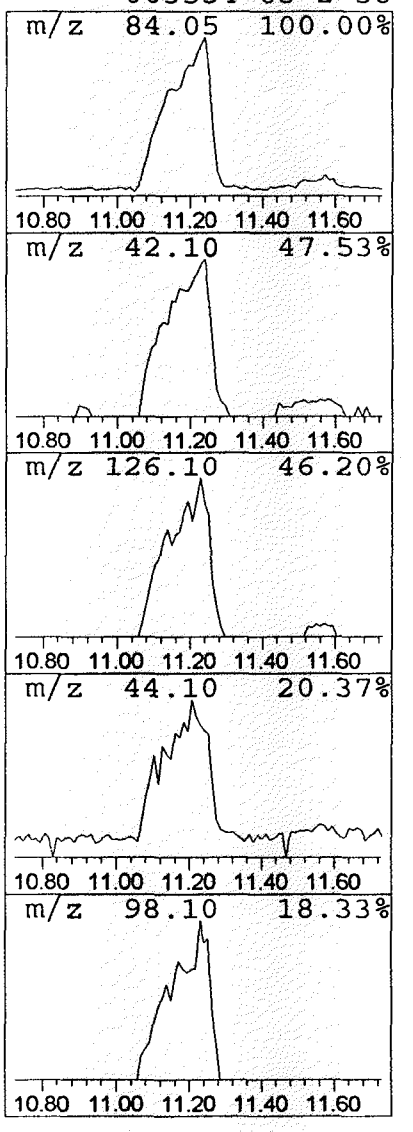
****

Peak Number 3 4H-1,2,4-Triazol-3-amine, 4... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.23	1.53 ug/L	666622	1,4-Dichlorobenzene-d4	9.71

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1,2,4-Triazol-3-amine, 4-prop...	126	C5H10N4	058661-97-5	47
2	Acetonitrile, (dimethylamino)- (...	84	C4H8N2	000926-64-7	43
3	Acetamide, N-formyl-N-[4-(1-form...	268	C13H20N2O4	054966-13-1	38
4	2-Pyrrolidinemethanol, 1-methyl-	115	C6H13NO	003554-65-2	38





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

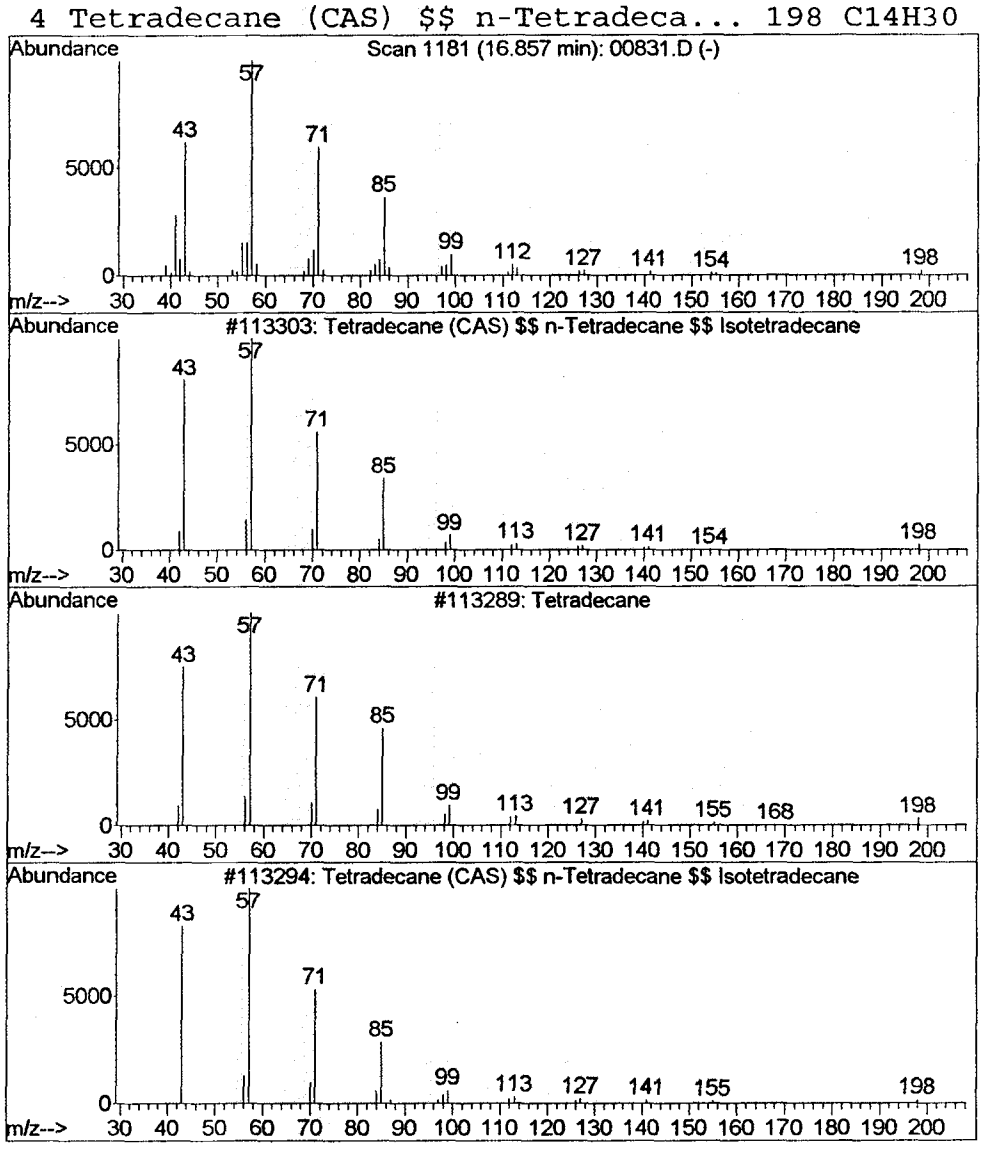
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

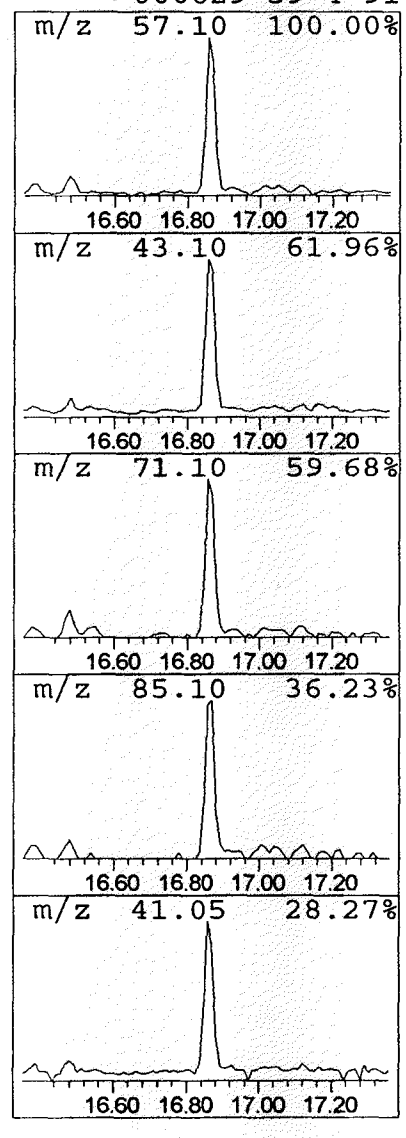
****

Peak Number 4 Tetradecane (CAS) $$ n-Tetr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.86	0.52 ug/L	349764	Acenaphthene-d10	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane (CAS) $$ n-Tetradeca...	198	C14H30	000629-59-4	96
2	Tetradecane	198	C14H30	000629-59-4	95
3	Tetradecane (CAS) $$ n-Tetradeca...	198	C14H30	000629-59-4	93
4	Tetradecane (CAS) $$ n-Tetradeca...	198	C14H30	000629-59-4	91





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

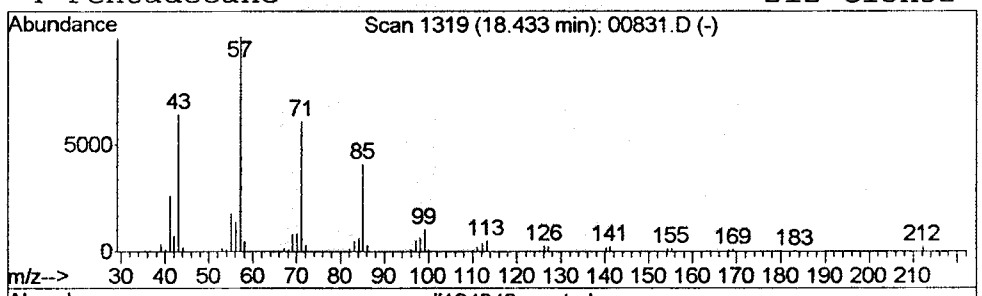
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

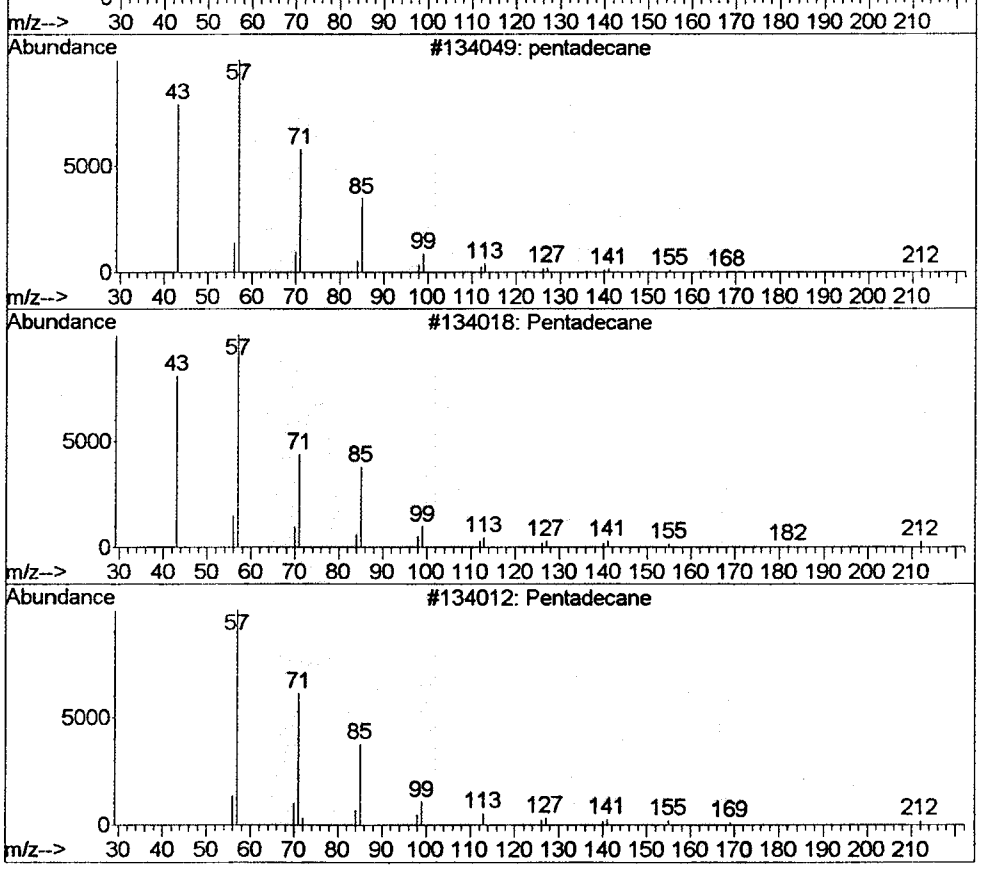
****

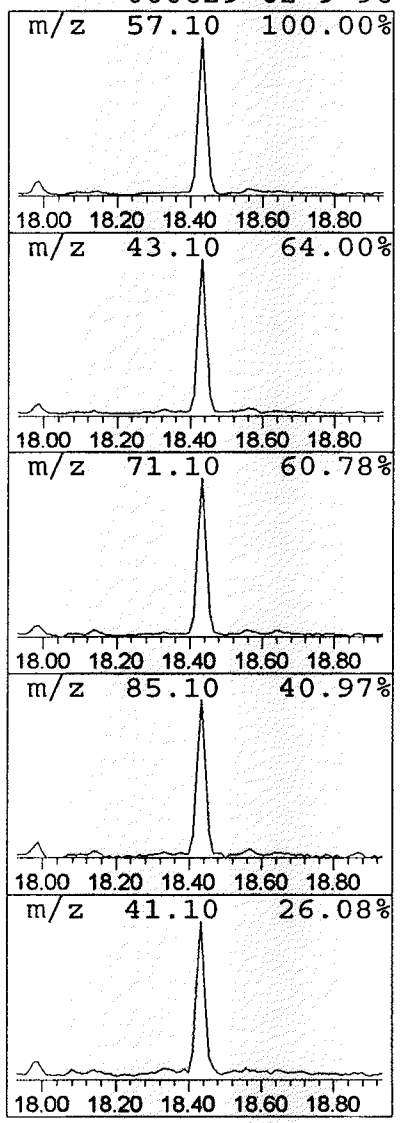
Peak Number 5 pentadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	1.24 ug/L	835359	Acenaphthene-d10	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	pentadecane	212	C15H32	000629-62-9	97
2	Pentadecane	212	C15H32	000629-62-9	96
3	Pentadecane	212	C15H32	000629-62-9	96
4	Pentadecane	212	C15H32	000629-62-9	96







Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

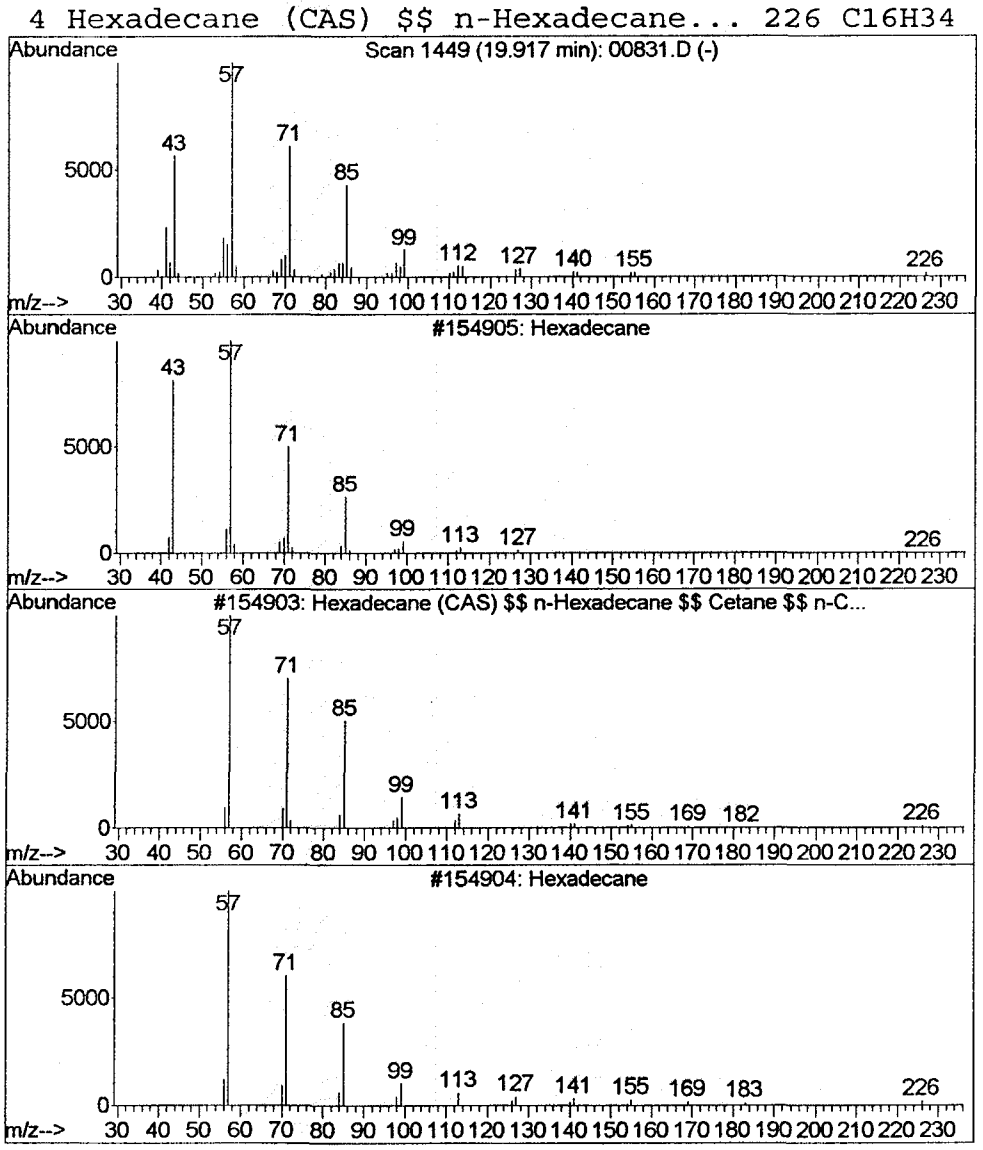
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

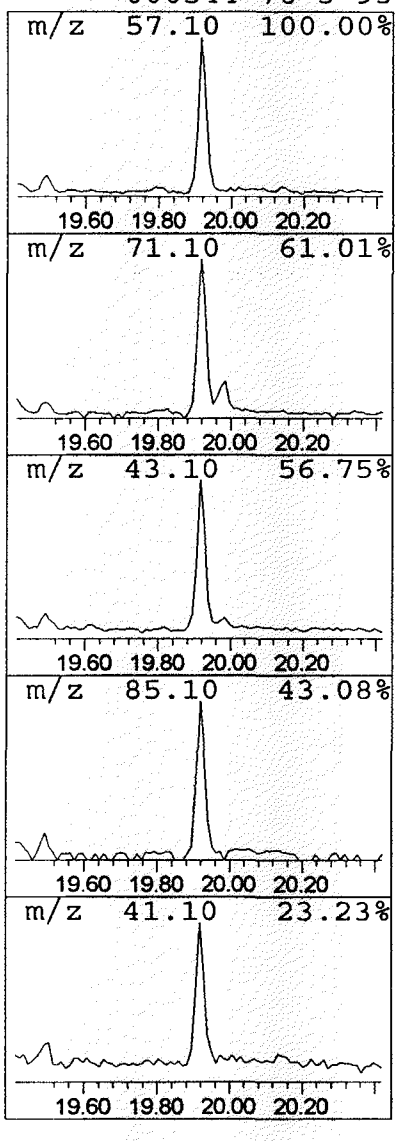
****

Peak Number 6 Hexadecane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	0.41 ug/L	278644	Acenaphthene-d10	18.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	94
2	Hexadecane (CAS) $$ n-Hexadecane...	226	C16H34	000544-76-3	93
3	Hexadecane	226	C16H34	000544-76-3	93
4	Hexadecane (CAS) $$ n-Hexadecane...	226	C16H34	000544-76-3	93





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

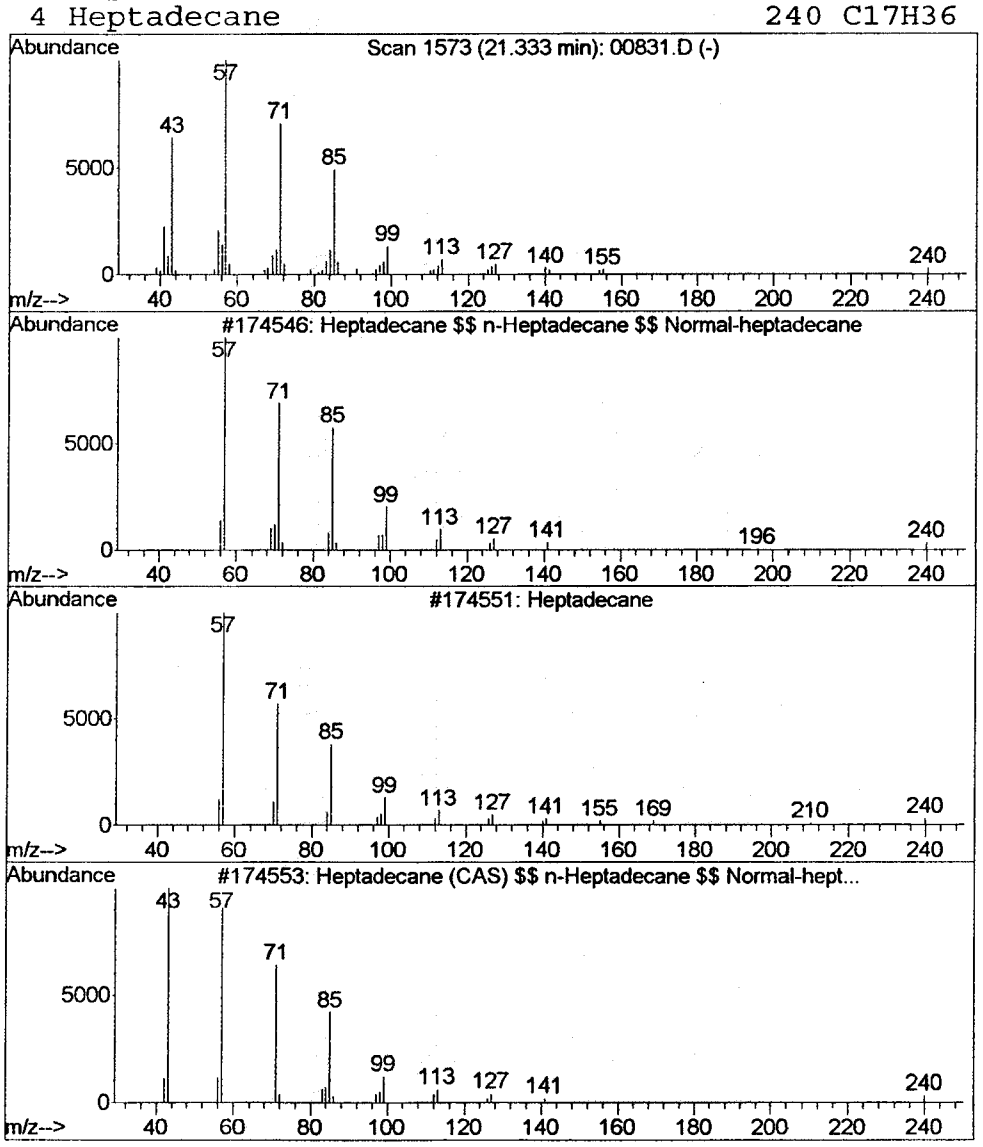
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

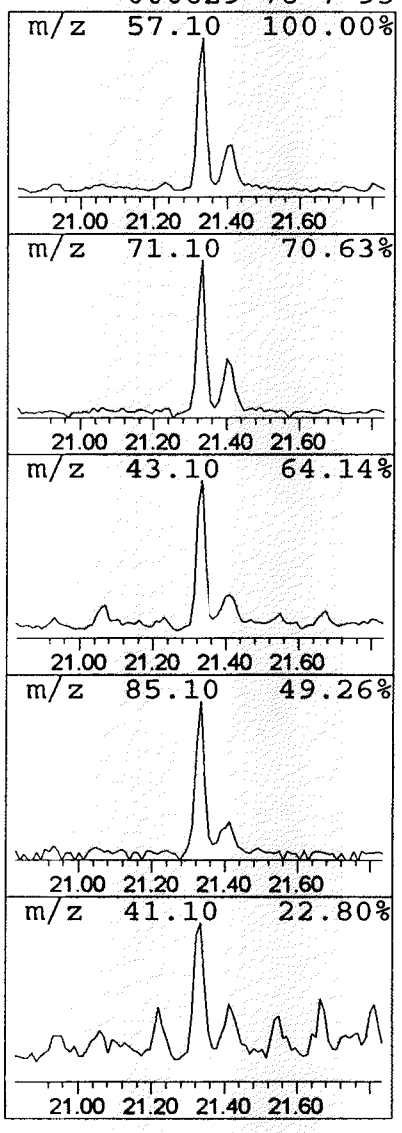
****

Peak Number 7 Heptadecane $$ n-Heptadecan... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	0.35 ug/L	251890	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane $$ n-Heptadecane $$ ...	240	C17H36	000629-78-7	97
2	Heptadecane	240	C17H36	000629-78-7	96
3	Heptadecane (CAS) $$ n-Heptadeca...	240	C17H36	000629-78-7	95
4	Heptadecane	240	C17H36	000629-78-7	93





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

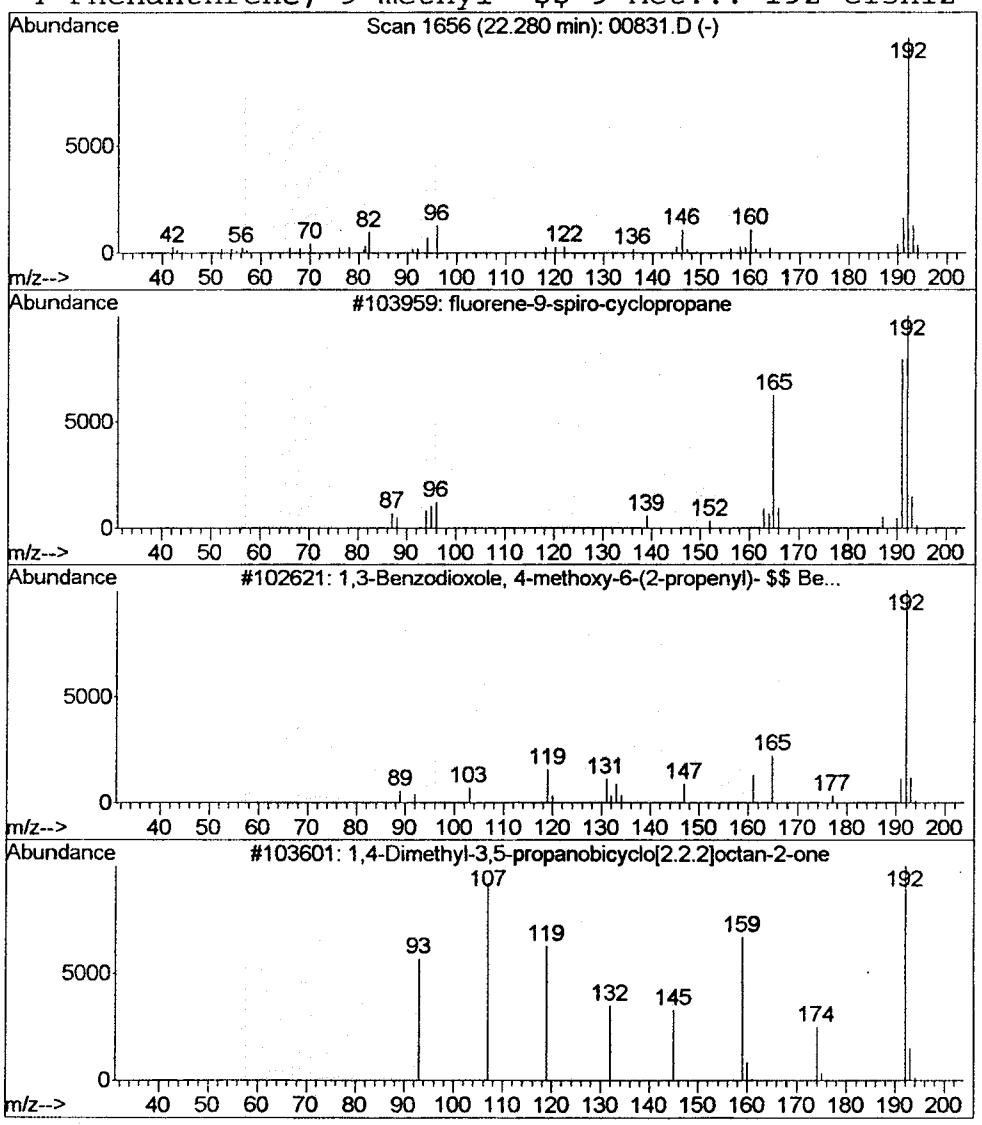
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

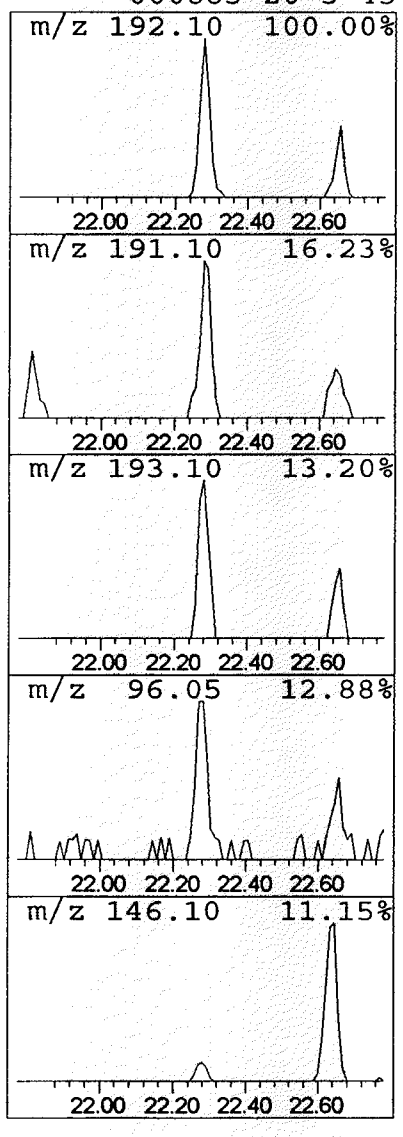
****

Peak Number 8 fluorene-9-spiro-cyclopropane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.41 ug/L	297073	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	fluorene-9-spiro-cyclopropane	192	C15H12	000000-00-0	59
2	1,3-Benzodioxole, 4-methoxy-6-(2...	192	C11H12O3	000607-91-0	58
3	1,4-Dimethyl-3,5-propanobicyclo[...	192	C13H20O	000000-00-0	49
4	Phenanthrene, 9-methyl- $$ 9-Met...	192	C15H12	000883-20-5	45





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

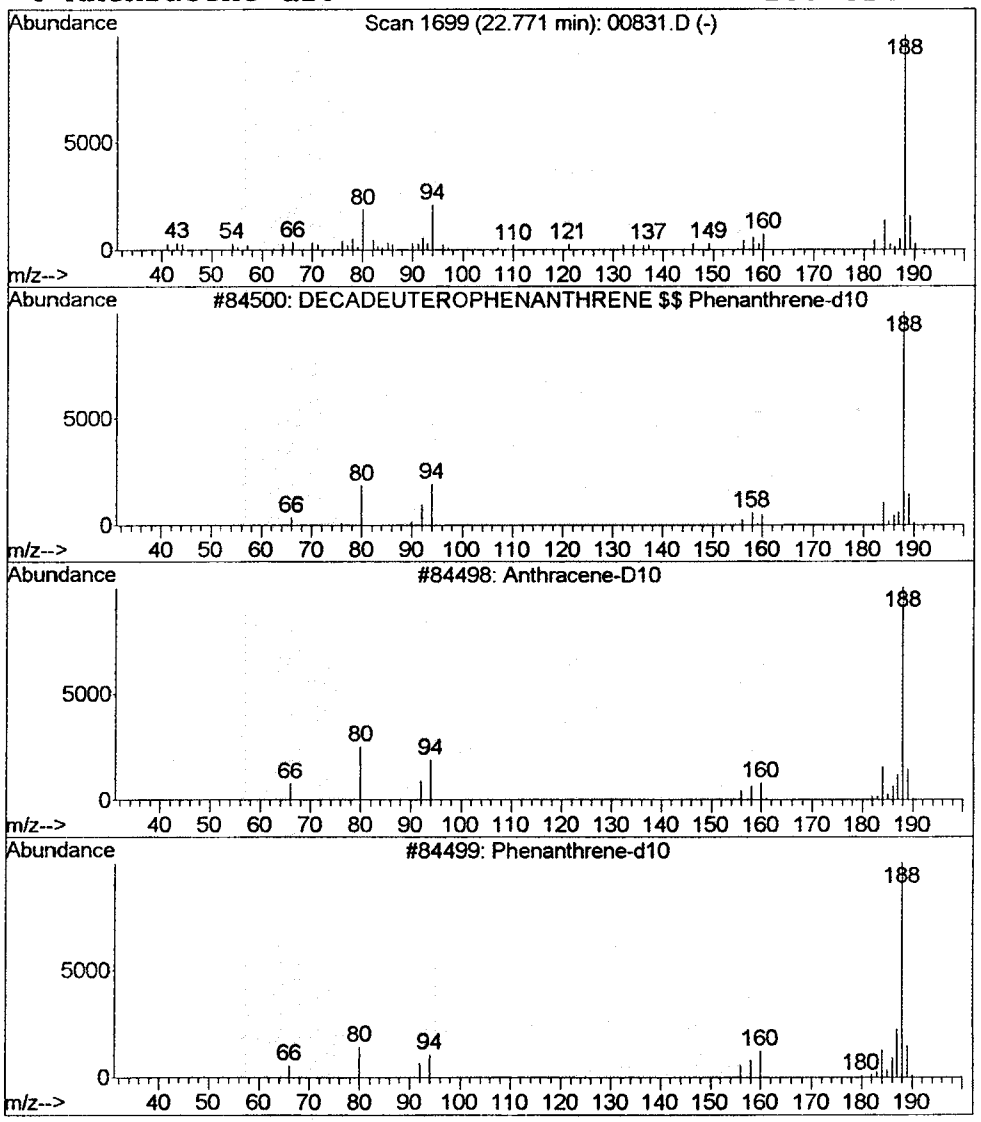
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

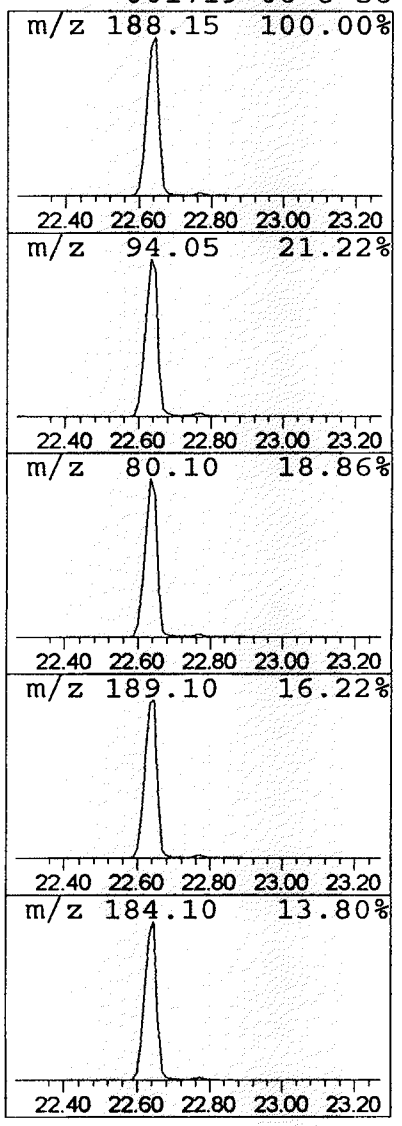
****

Peak Number 9 DECADEUTEROPHENANTHRENE $$ ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.47 ug/L	339091	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	90
2	Anthracene-D10	188	C14D10	000000-00-0	83
3	Phenanthrene-d10	188	C14D10	001517-22-2	72
4	Anthracene-d10-	188	C14D10	001719-06-8	56





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

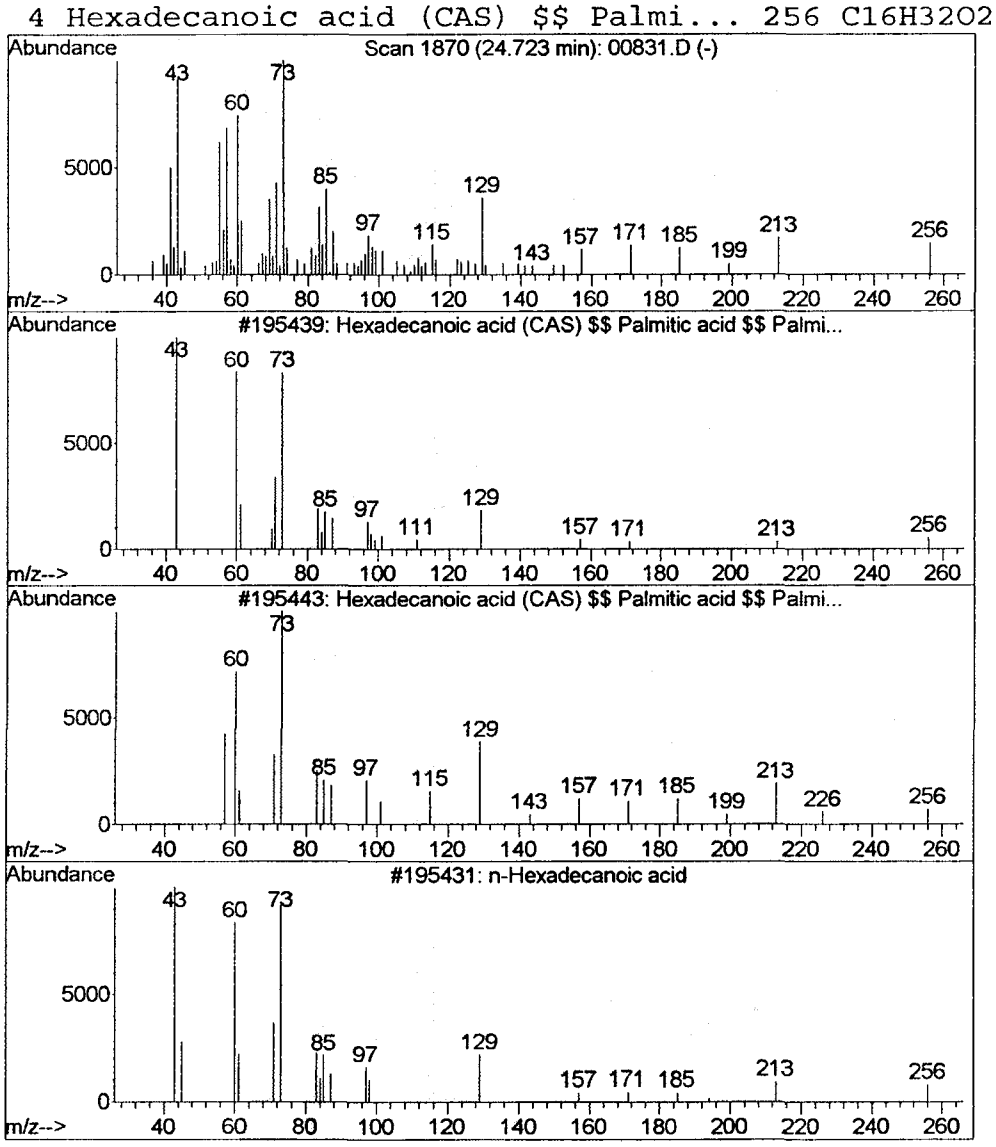
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

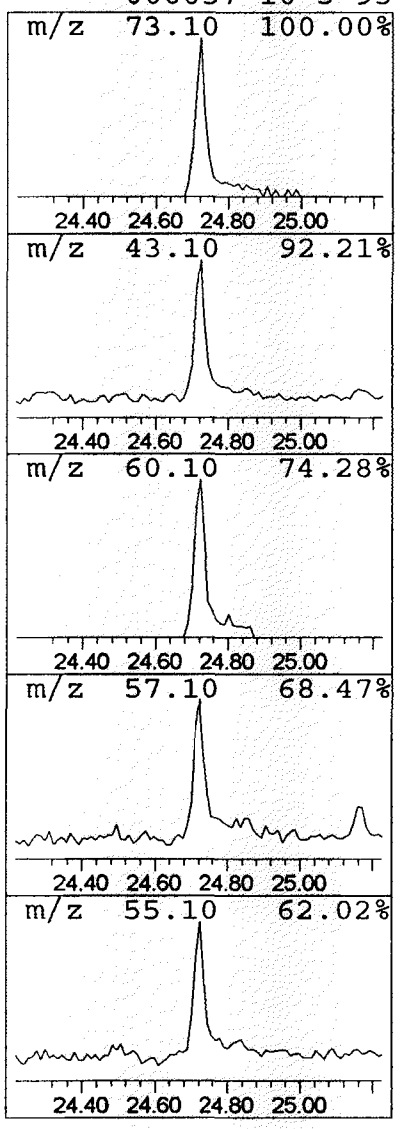
****

Peak Number 10 Hexadecanoic acid (CAS) $$ ... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.72	0.44 ug/L	322072	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid (CAS) $$ Palmi...	256	C16H32O2	000057-10-3	98
2	Hexadecanoic acid (CAS) $$ Palmi...	256	C16H32O2	000057-10-3	97
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Hexadecanoic acid (CAS) $$ Palmi...	256	C16H32O2	000057-10-3	93





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : January 31, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

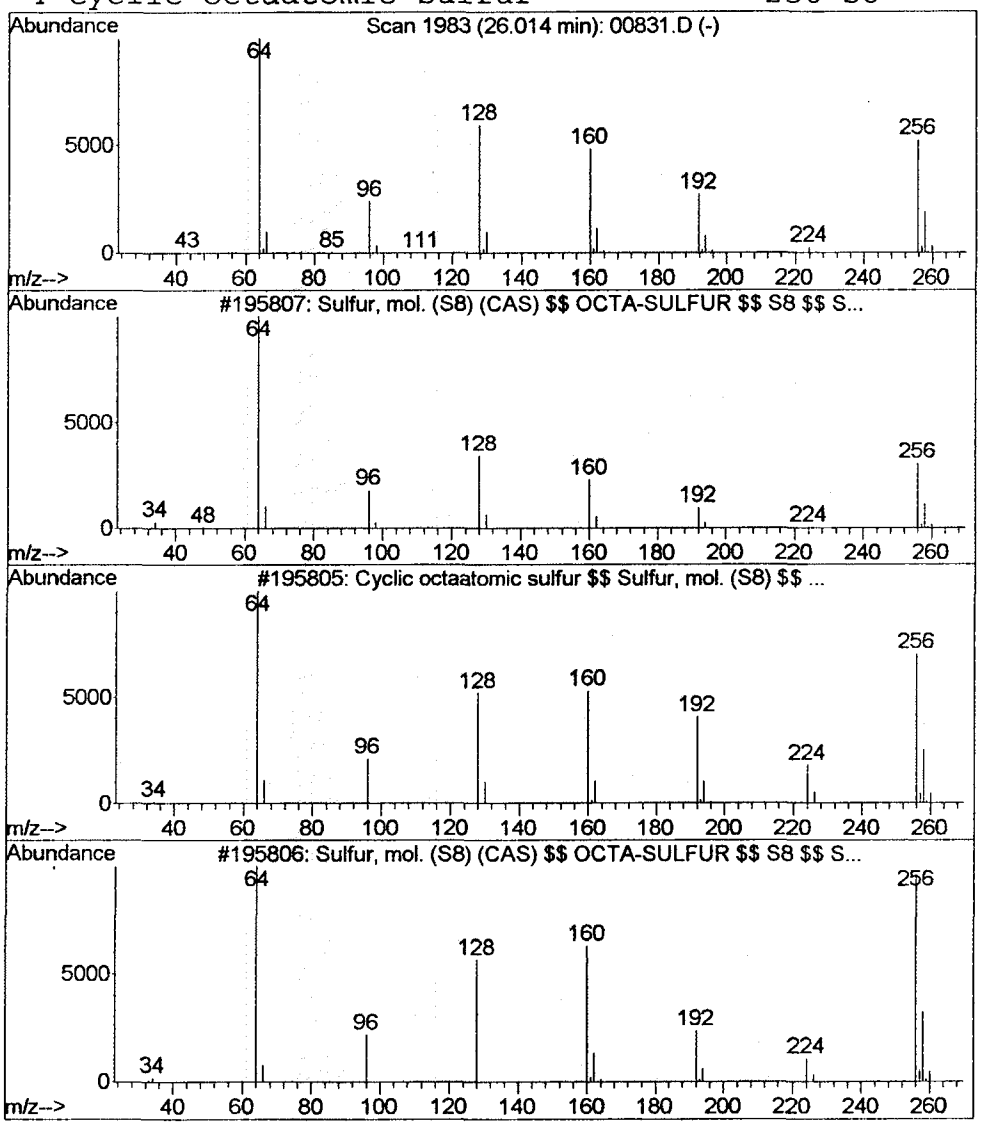
Quant Method : C:\MSDCHEM\1...\SCAN508.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

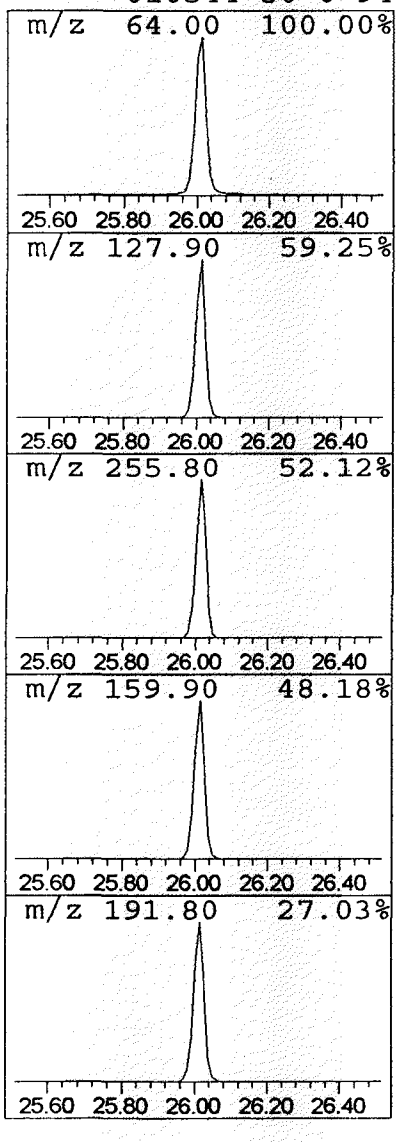
****

Peak Number 11 Sulfur, mol. (S8) (CAS) $$ ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.01	1.74 ug/L	1260700	Phenanthrene-d10	22.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	97
2	Cyclic octaatomic sulfur $$ Sulf...	256	S8	010544-50-0	95
3	Sulfur, mol. (S8) (CAS) $$ OCTA-...	256	S8	010544-50-0	95
4	Cyclic octaatomic sulfur	256	S8	010544-50-0	94





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D
Acq On : 31 Jan 2002 1:01 pm
Sample : 508 scan
Misc : January 31, 2002
MS Integrat[illegible] Params: LSCINT.P

Vial: 4
Operator:
Inst : Instrumen
Multiplr: 1.00

Quant Methc
Title
Library

DERIVATIVE OF CHOLESTEROL

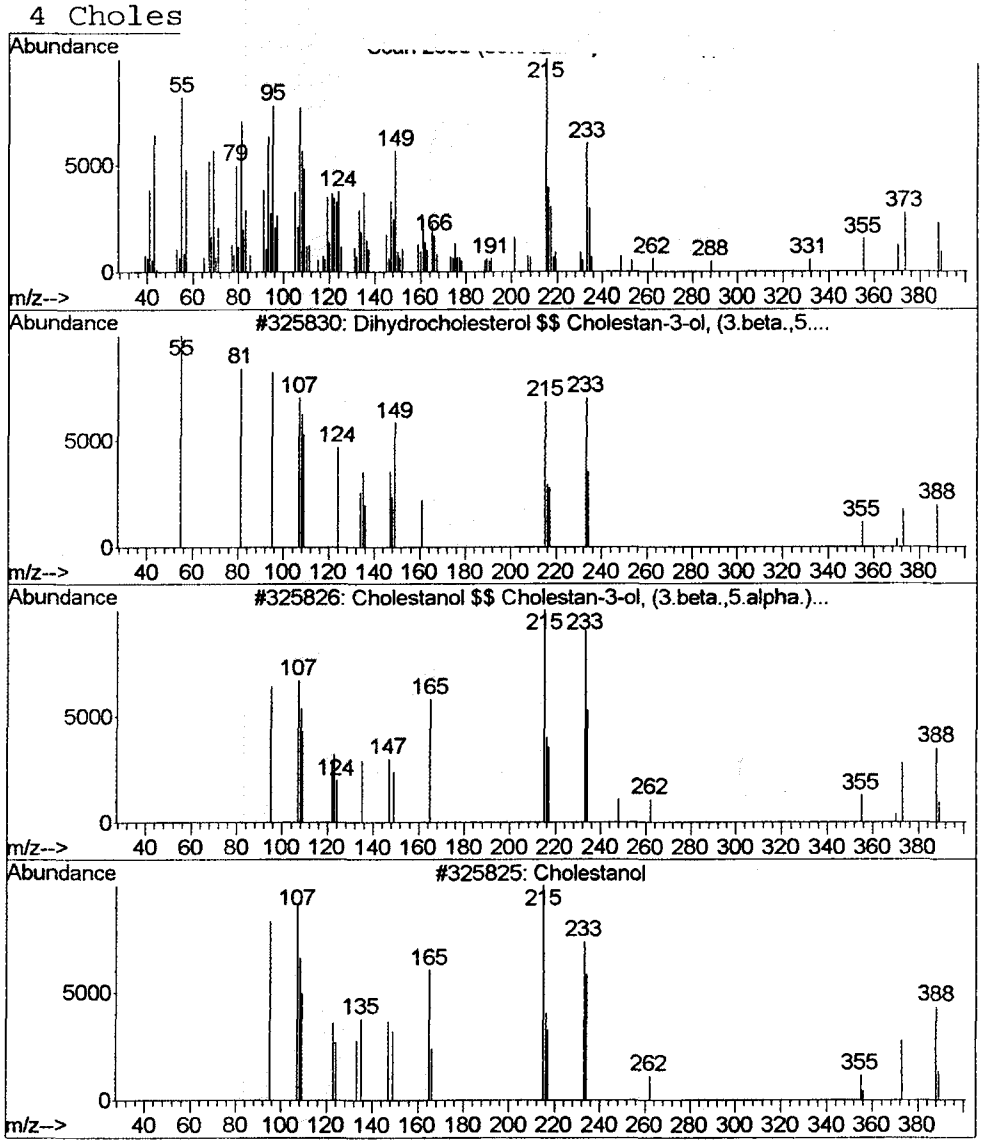
3.β,5α - CHOLESTAN-3-OL

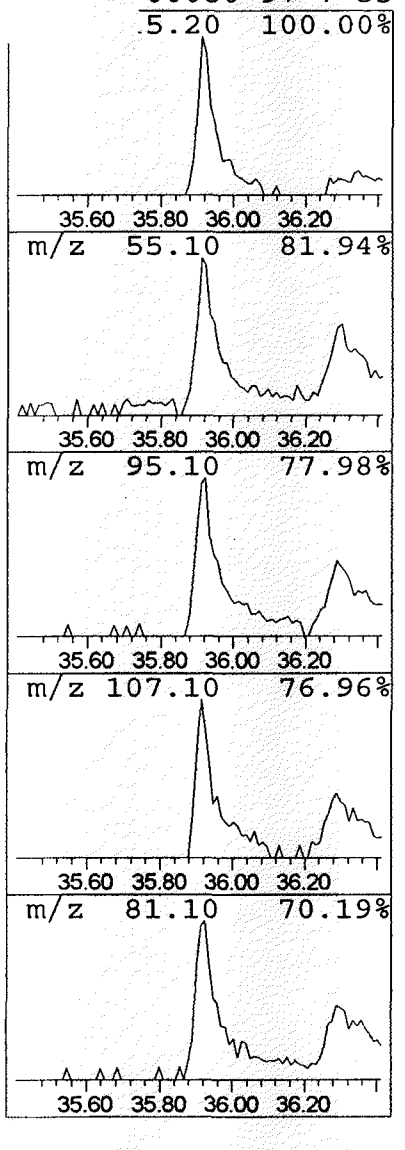
****
Peak Numbe

****
on Rank 2

R.T.		R.T.
35.91		34.42

Hit# of		AS#	Qual
1	Dihydr	00080-97-7	99
2	Choles	00080-97-7	93
3	Choles	00080-97-7	70
4	Choles	00080-97-7	55





Library Search Compound Report

Data File : C:\MSDCHEM\1\5973N\02JAN31\00831.D Vial: 4
Acq On : 31 Jan 2002 1:01 pm Operator:
Sample : 50 Inst : Instrumen
Misc : Ja .00
MS Integration

Quant Method :
Title :
Library :

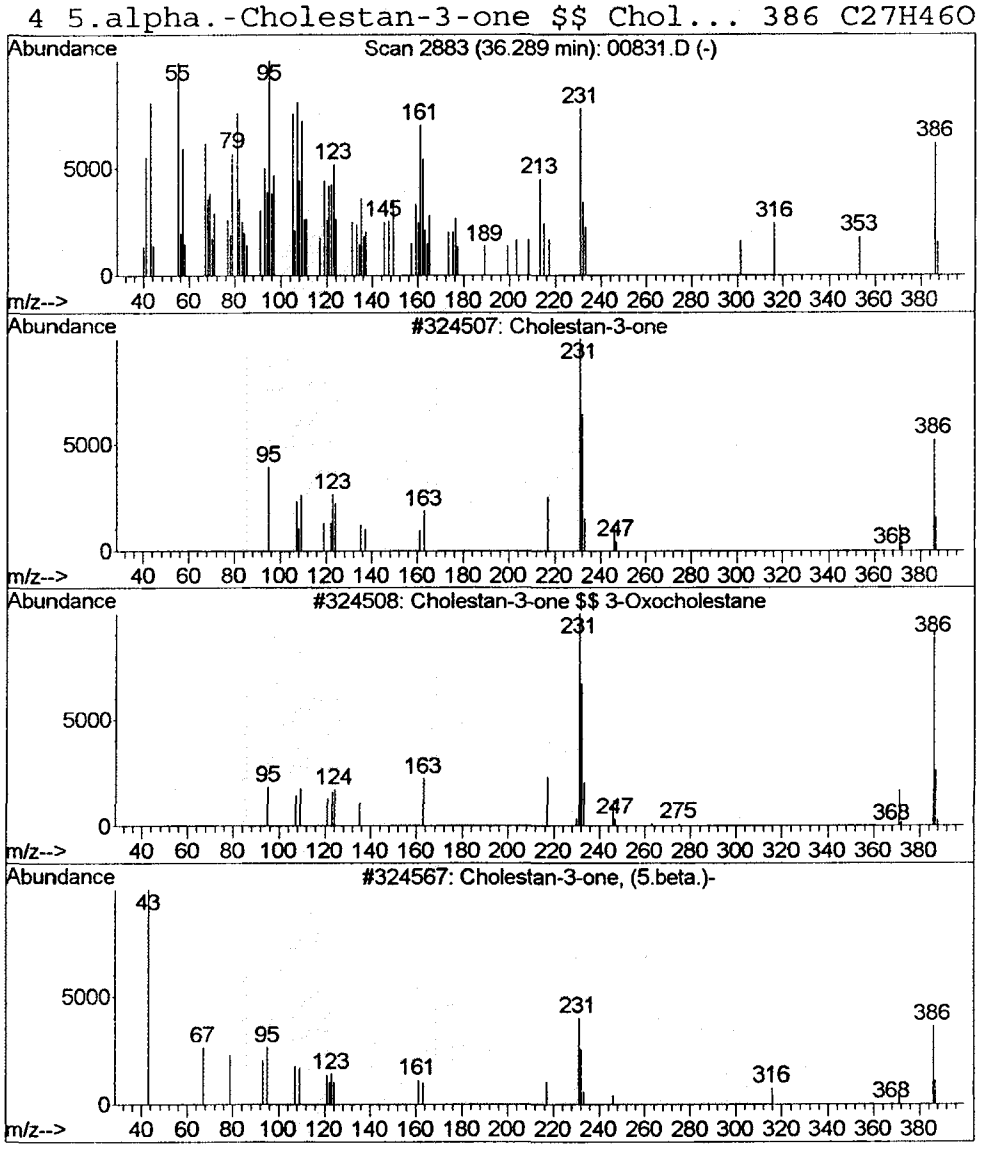
DERIVATIVE OF CHOLESTEROL

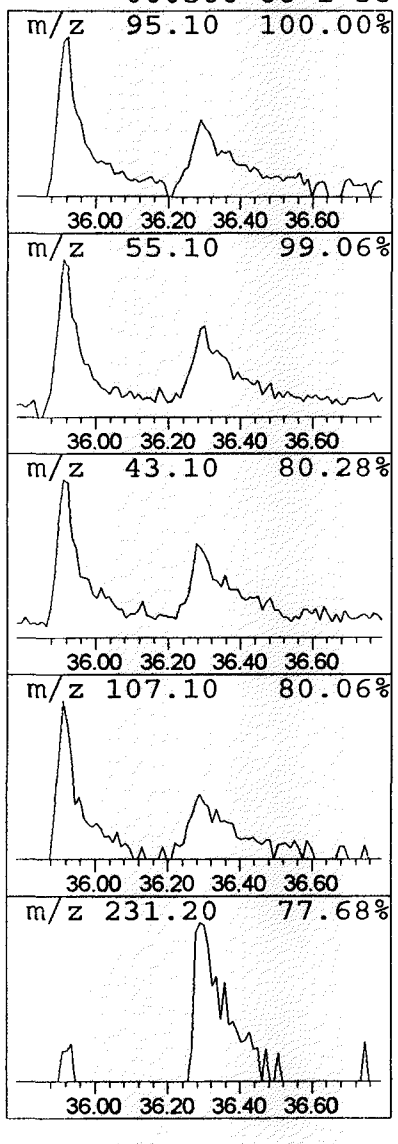
********** *******
Peak Number 1 Rank 6

R.T.	Est(	R.T.
36.29	1.:	34.42

Hit# of 5

		Qual
1	Cholestan	00-08-5 43
2	Cholestan	00-08-5 43
3	Cholestan-3-one, (5.beta.)	01-53-6 42
4	5.alpha.-Cholestan-3-one $$ Chol... 386 C27H46O	000566-88-1 38





Tentatively Identified Compound (LSC) summary

Operator ID: Date Acquired: 31 Jan 2002 1:01 pm
Data File: C:\MSDCHEM\1\5973N\02JAN31\00831.D
Name: 508 scan
Misc: January 31, 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
2-Pentanone, 4-hy...	6.02	1.2	ug/L	515800	1	9.71	8730680	20.0
2-Pentanone, 4-am...	6.68	3.3	ug/L	1457280	1	9.71	8730680	20.0
4H-1,2,4-Triazol-...	11.23	1.5	ug/L	666622	1	9.71	8730680	20.0
Tetradecane (CAS)...	16.86	0.5	ug/L	349764	3	18.34	13503000	20.0
pentadecane	18.43	1.2	ug/L	835359	3	18.34	13503000	20.0
Hexadecane	19.92	0.4	ug/L	278644	3	18.34	13503000	20.0
Heptadecane $$ n-...	21.33	0.3	ug/L	251890	4	22.65	14480200	20.0
fluorene-9-spiro-...	22.28	0.4	ug/L	297073	4	22.65	14480200	20.0
DECADEUTERORHENAN...	22.77	0.5	ug/L	339091	4	22.65	14480200	20.0
Hexadecanoic acid...	24.72	0.4	ug/L	322072	4	22.65	14480200	20.0
Sulfur, mol. (S8)...	26.01	1.7	ug/L	1260700	4	22.65	14480200	20.0
Dihydrocholestero..	35.91	1.7	ug/L	1011280	6	34.42	11563300	20.0
Cholestan-3-one	36.29	1.2	ug/L	703734	6	34.42	11563300	20.0