User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 02/27/2002 Time: 09:03:09

Sample: AE01141
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 2/27/02 09:02 Ended: 2/27/02 09:02 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		94		5.0

FB 1047 / 1002 pending

ID 44450 / 01446

Call 1/14/02 by Dessources

CAS 4813-57-4

90/100

acrylic acid octadecanoyl ester

WB

called Dr. Hurley 3/1/2

9:30

composed of wax - not a natural product

Comments for Sample AE01141 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 02-27-2002 Time: 09:05:46

The GCMS scan, from 35 to 550 amu, reveals the presence of Acrylic acid octadecanyl ester at an estimated level of 0.44 ug/L and with a fit of 90 out of 100. The recoveries for 16 of the 43 compounds in the LCS Standard were above their acceptance ranges, while 3 of the 43 compounds were below their acceptance ranges.

Data File : C:\MSDCHEM\1\5973N\02FEB25\01141.D Vial: 7
Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 26 08:28:40 2002 Quant Results File: HP022102.RES

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Last Update : Mon Feb 25 10:47:59 2002
Response via : Initial Calibration
DataAcq Meth : HP020702

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.72	152	1506257	20.00	ug/L	0.00
10) Naphthalene-d8	13.19	136	6549104	20.00	ug/L	0.00
17) Acenaphthene-d10	18.33	164	3276500	20.00	ug/L	0.00
29) Phenanthrene-d10	22.63	188	5348304	20.00	ug/L	-0.01
38) Chrysene-d12	30.49	240	4185543	20.00	ug/L	-0.03
44) Perylene-d12	34.41	264	2813341	20.00	ug/L	-0.04
System Monitoring Compounds						
37) 2,4-DDD	27.72	235	335876	4.71	ug/L	0.00
Spiked Amount 5.000			Recovery = 94.20%			
Target Compounds						Qvalue
20) Dimethylphthalate	18.34	163	528939	2.66	ug/L #	57
21) 2,6-Dinitrotoluene	18.33	165	416677	9.08	ug/L #	27

(#) = qualifier out of range (m) = manual integration
01141.D HP022102.M Tue Feb 26 08:28:41 2002 Page 1

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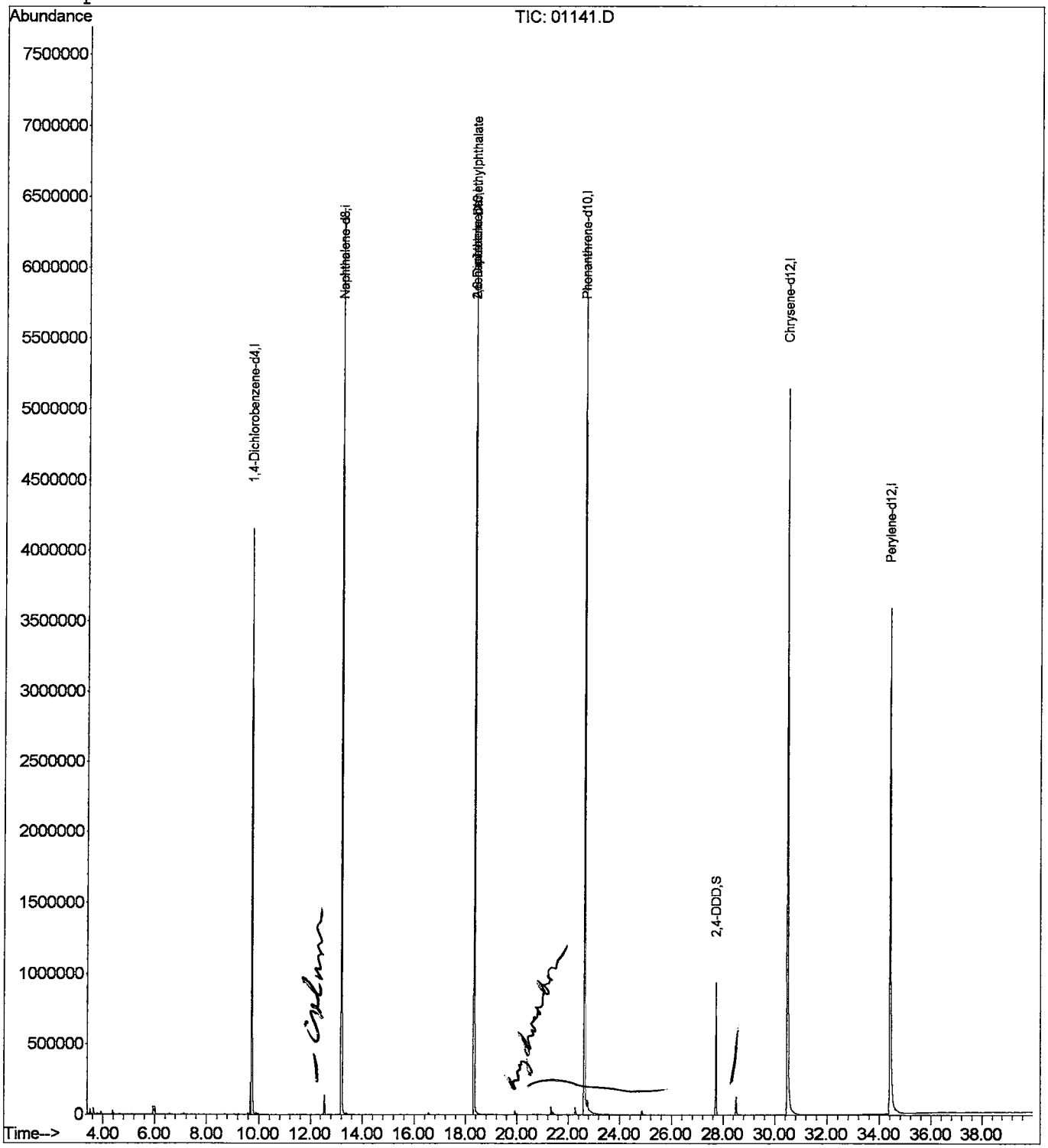
Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: SPLIT.P
Quant Time: Feb 26 8:28 2002 Quant Results File: HP022102.R

Method : C:\MSDCHEM\1\METHODS\METHODS\HP022102.M (RTE Integrator)
Title : 508 scan method
Last Update : Mon Feb 25 10:47:59 2002
Response via : Initial Calibration



Data File : C:\MSDCHEM\1\5973N\02FEB25\01141.D Vial: 7
Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Method : C:\MSDCHEM\1\METHODS\METHODS\HP022102.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

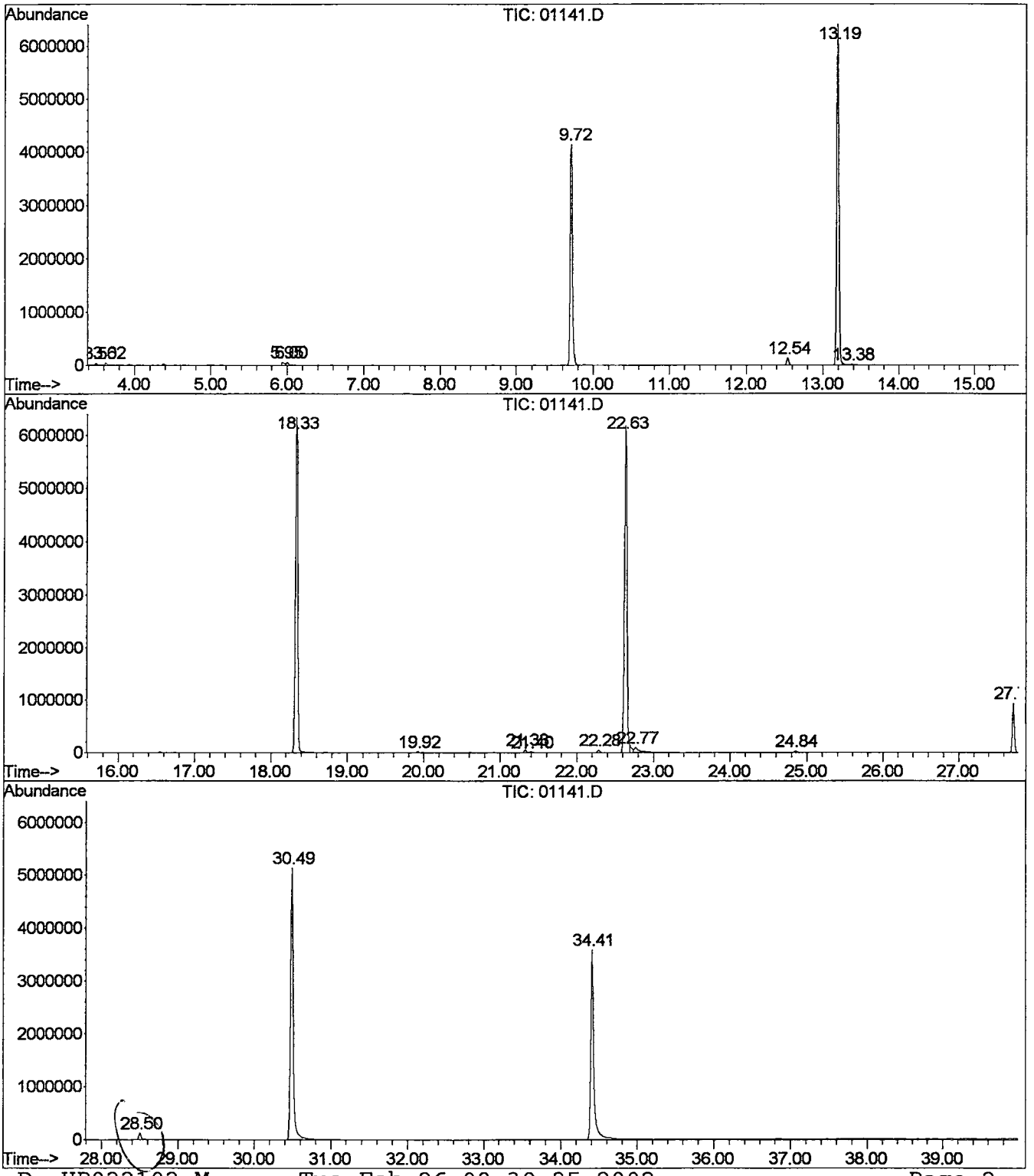
If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.498	7	11	15	rBV	37768	53929	0.38%	0.073%
2	3.622	19	22	33	rVB	42232	66250	0.47%	0.090%
3	5.947	225	228	231	rBV	58024	138149	0.99%	0.188%
4	6.004	231	233	249	rVV	55416	127618	0.91%	0.174%
5	9.718	557	562	567	rBV	4150801	8356122	59.62%	11.361%
6	12.540	807	812	817	rBV	135227	227463	1.62%	0.309%
7	13.195	865	870	875	rBV	6413136	12372702	88.28%	16.822%
8	13.375	883	886	895	rVB3	13655	39172	0.28%	0.053%
9	18.331	1319	1325	1331	rBV	6339389	13374387	95.43%	18.184%
10	19.923	1461	1466	1469	rBV	26247	46412	0.33%	0.063%
11	21.334	1587	1591	1595	rBV	54633	106215	0.76%	0.144%
12	21.402	1595	1597	1601	rVV2	17133	38789	0.28%	0.053%
13	22.282	1671	1675	1679	rVV2	47562	88340	0.63%	0.120%
14	22.632	1701	1706	1711	rBV2	6185173	14014753	100.00%	19.055%
15	22.768	1715	1718	1739	rVB	90277	403812	2.88%	0.549%
16	24.845	1897	1902	1913	rBV	28297	66372	0.47%	0.090%
17	27.724	2153	2157	2163	rBV	939831	1639868	11.70%	2.230%
18	28.503	2221	2226	2241	rVB	126391	273811	1.95%	0.372%
19	30.489	2397	2402	2443	rBV	5142408	12419300	88.62%	16.886%
20	34.407	2743	2749	2781	rBV	3584984	9696527	69.19%	13.184%

Sum of corrected areas: 73549991

File : C:\MSDCHEM\1\5973N\02FEB25\01141.D
Operator :
Acquired : 25 Feb 2002 4:11 pm using AcqMethod HP020702
Instrument : Instrumen
Sample Name: 508 scan
Misc Info : February 25, 2002
Vial Number: 7
Quant File :HP022102.RES (RTE Integrator)



Data File : C:\MSDCHEM\1\5973N\02FEB25\01141.D Vial: 7
Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

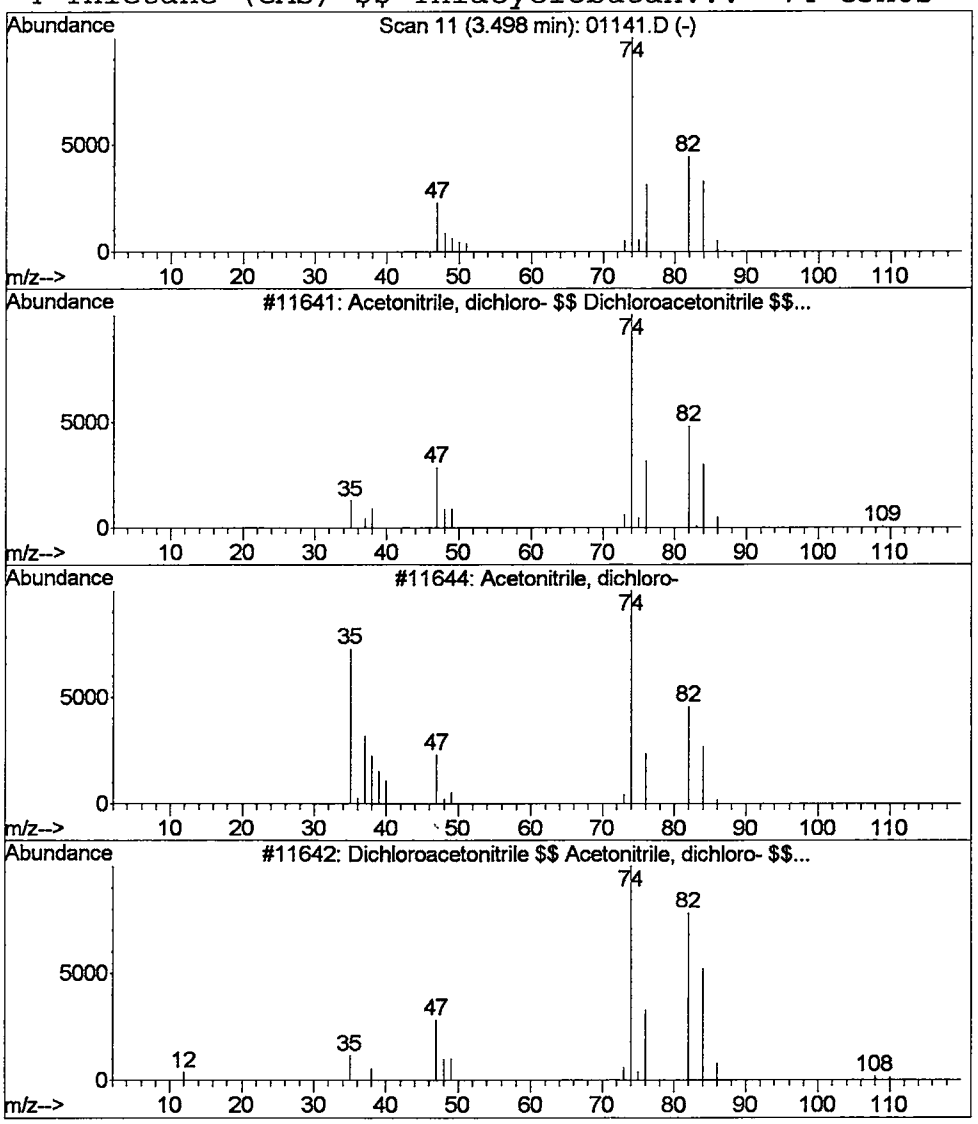
Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

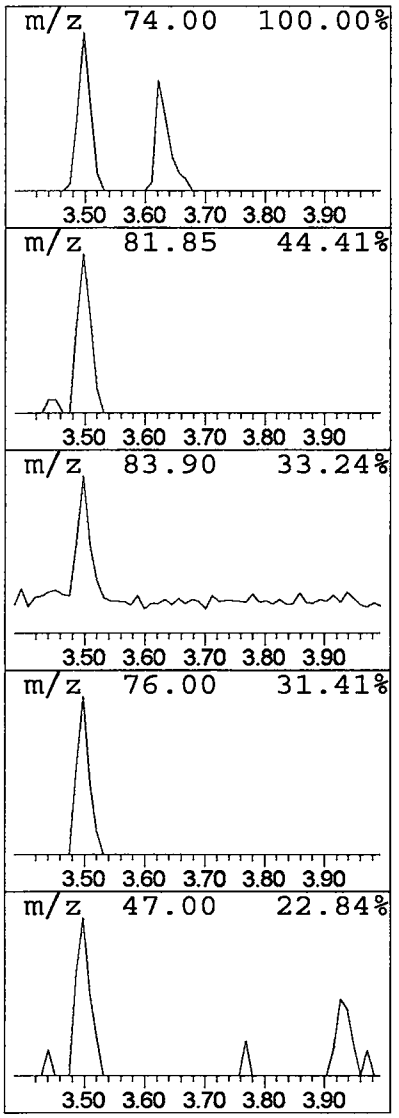
****

Peak Number 1 Acetonitrile, dichloro- $$ ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	0.13 ug/L	53929	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, dichloro- $$ Dichl...	109	C2HCl2N	003018-12-0	83
2	Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	78
3	Dichloroacetonitrile $$ Acetonit...	109	C2HCl2N	003018-12-0	64
4	Thietane (CAS) $$ Thiacyclobutan...	74	C3H6S	000287-27-4	37





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Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
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Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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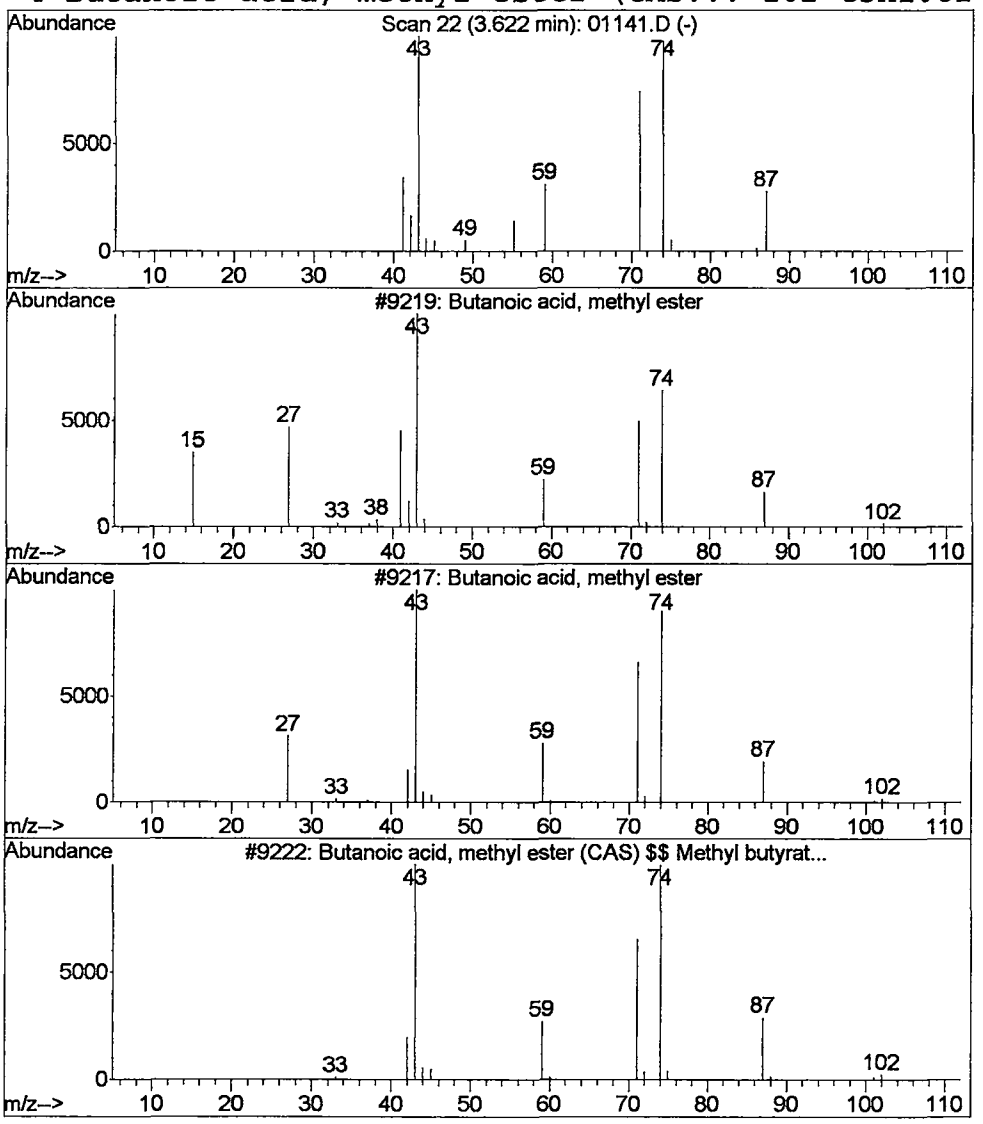
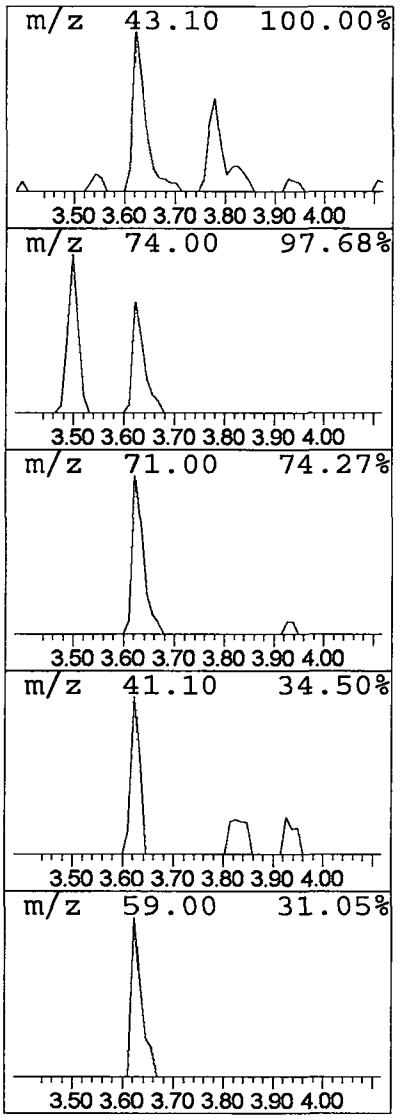
Peak Number 2 Butanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.62	0.16 ug/L	66250	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
3	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83
4	Butanoic acid, methyl ester (CAS...	102	C5H10O2	000623-42-7	83





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Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
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Library : C:\DATABASE\WILEY7N.L

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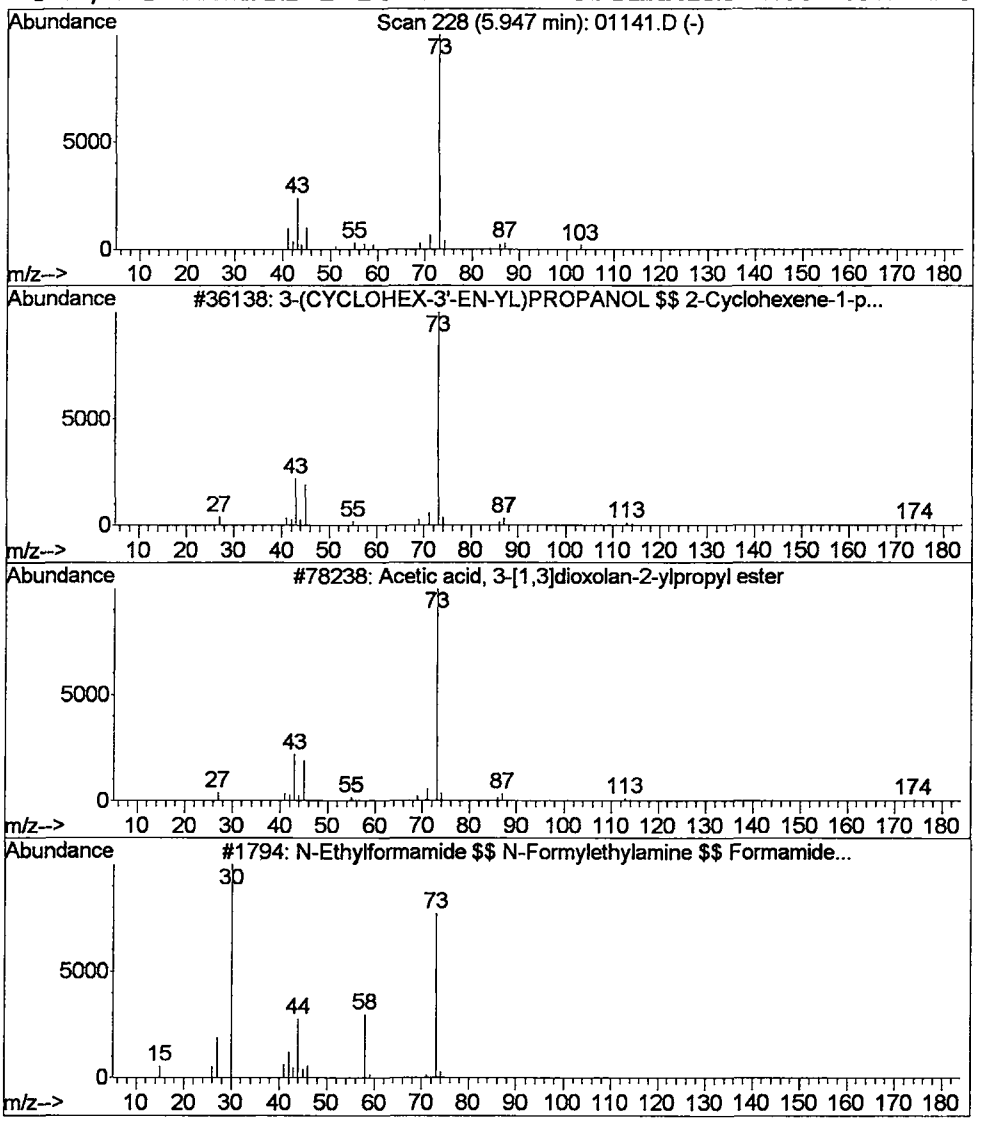
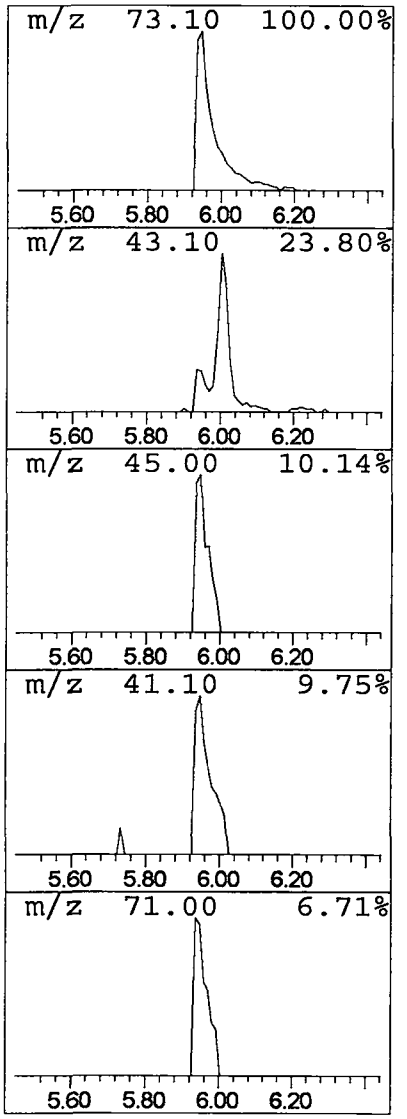
Peak Number 3 3-(CYCLOHEX-3'-EN-YL)PROPAN... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.95	0.33 ug/L	138149	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	42
2	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	42
3	N-Ethylformamide $$ N-Formylethy...	73	C3H7NO	000627-45-2	9
4	N,N-DIMETHYL-2-BUTOXYISOPROPYLAMINE	159	C9H21NO	000000-00-0	9





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Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
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Library : C:\DATABASE\WILEY7N.L

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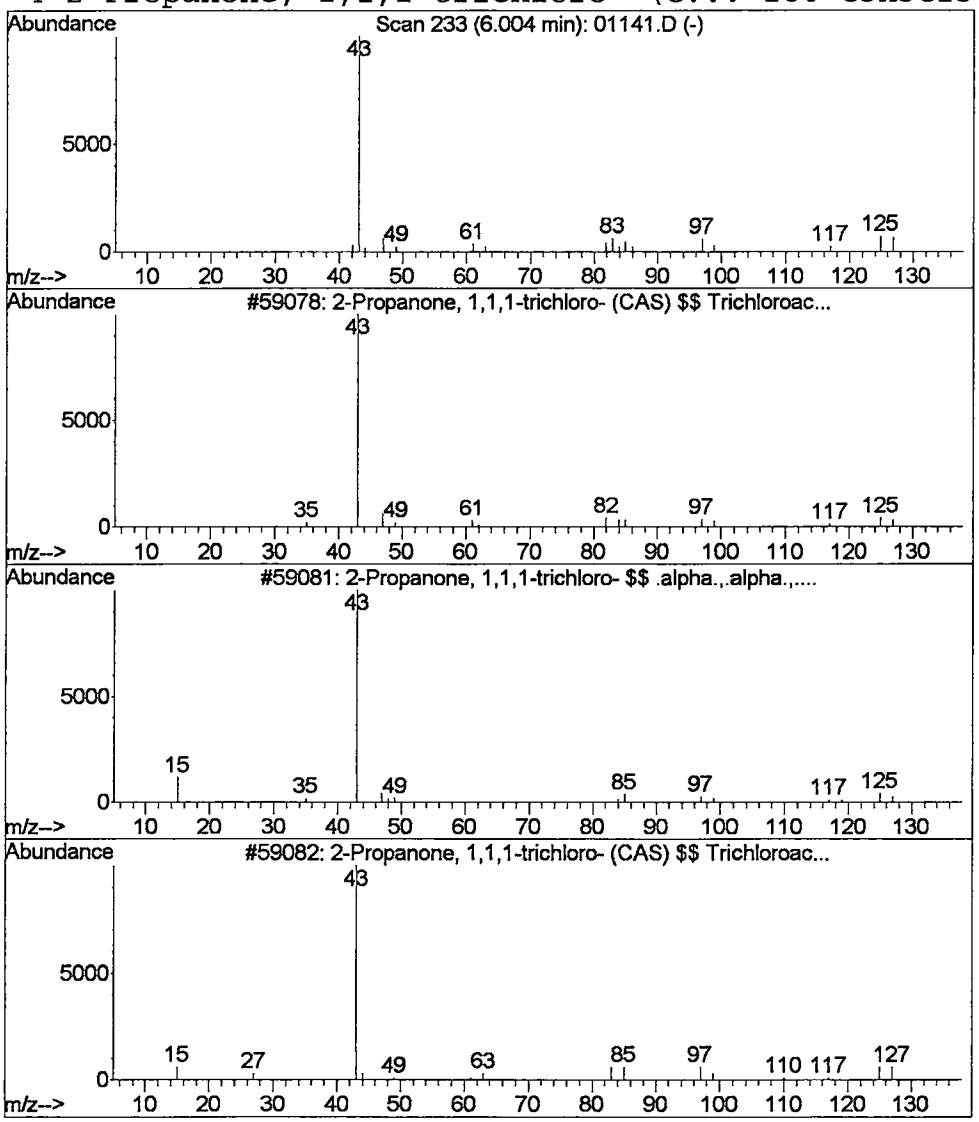
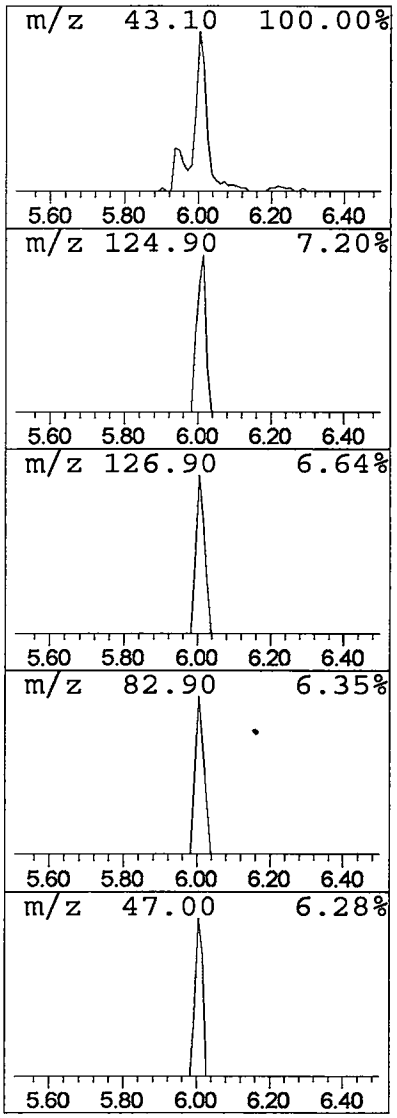
Peak Number 4 2-Propanone, 1,1,1-trichlor... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.00	0.31 ug/L	127618	1,4-Dichlorobenzene-d4	9.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	83
2	2-Propanone, 1,1,1-trichloro- $$...	160	C3H3Cl3O	000918-00-3	78
3	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	53
4	2-Propanone, 1,1,1-trichloro- (C...	160	C3H3Cl3O	000918-00-3	45





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Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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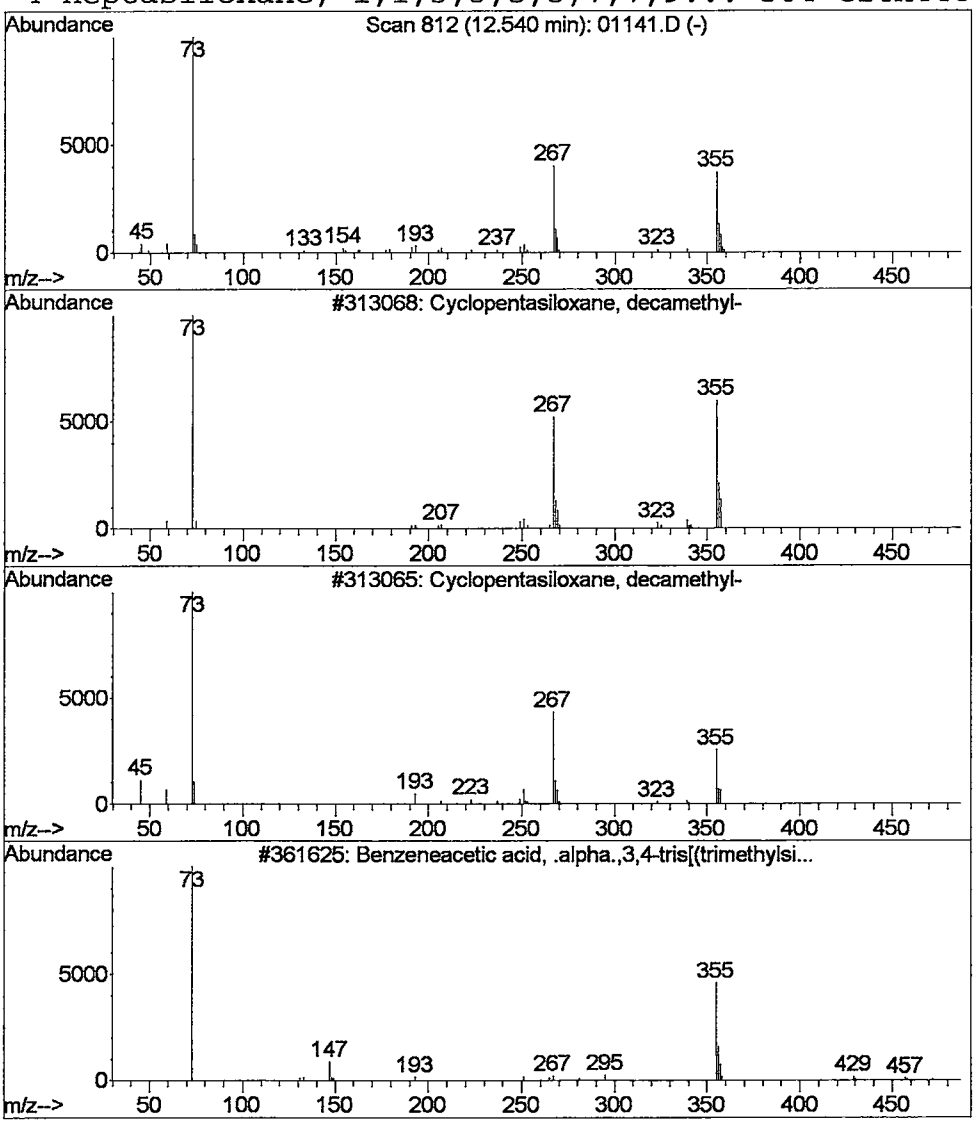
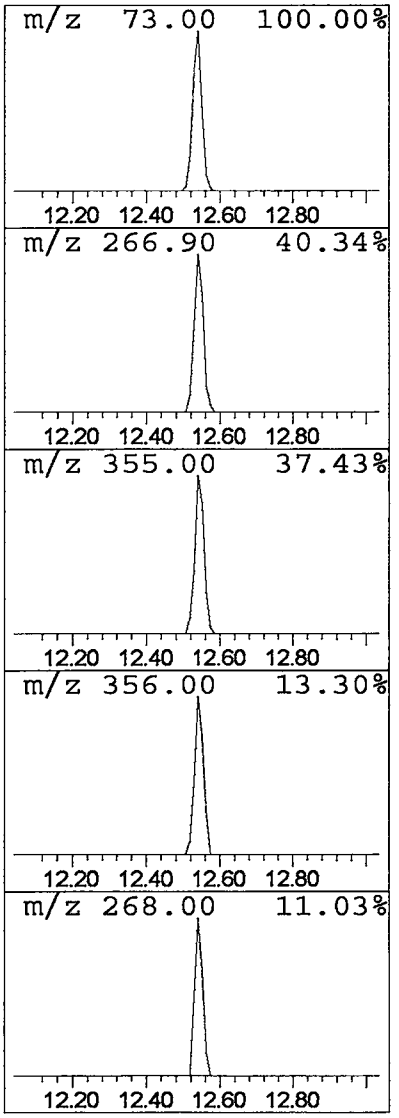
Peak Number 5 Cyclopentasiloxane, decamet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.54	0.37 ug/L	227463	Naphthalene-d8	13.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	80
2	Cyclopentasiloxane, decamethyl-	370	C10H30O5Si5	000541-02-6	53
3	Benzeneacetic acid, .alpha.,3,4-...	472	C20H40O5Si4	037148-65-5	38
4	Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	36





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Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
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Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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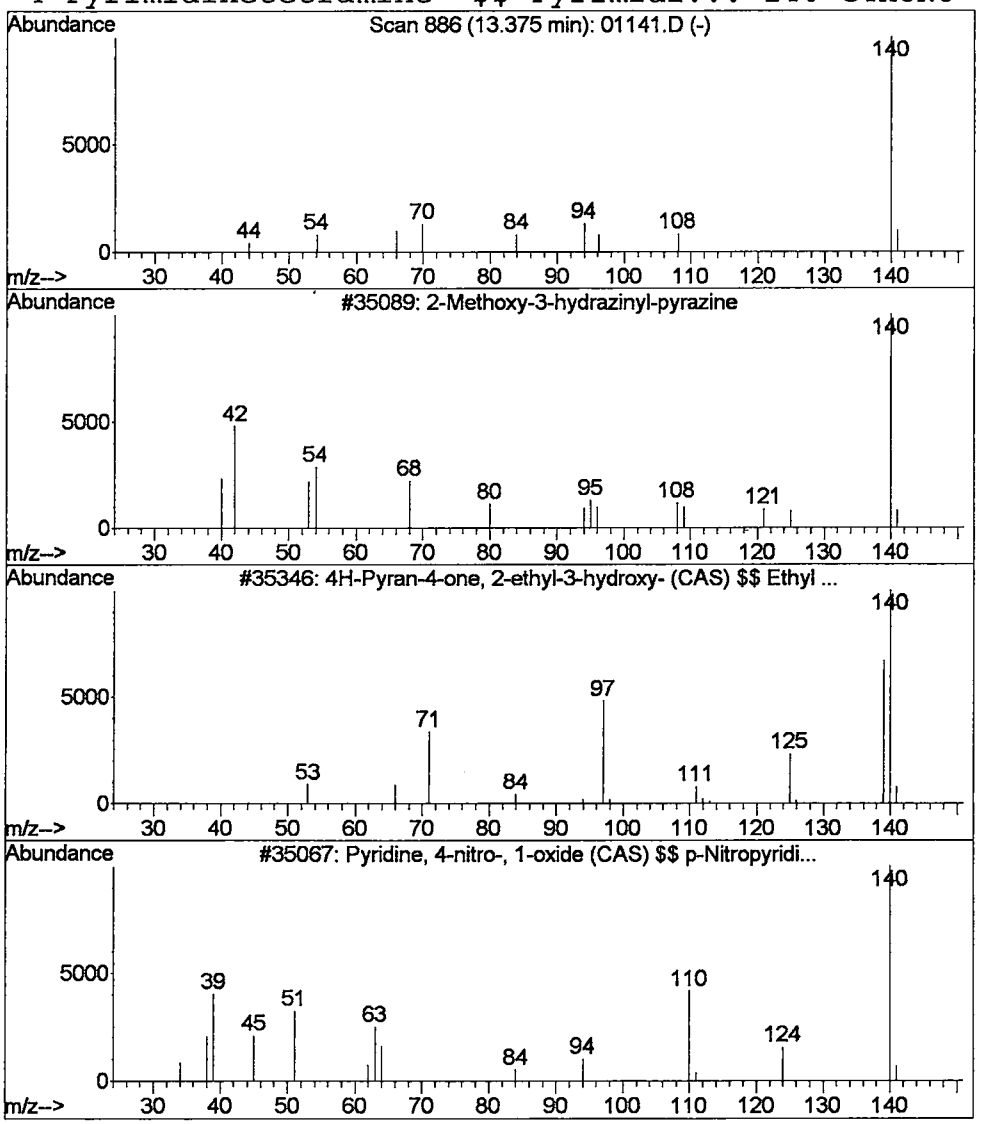
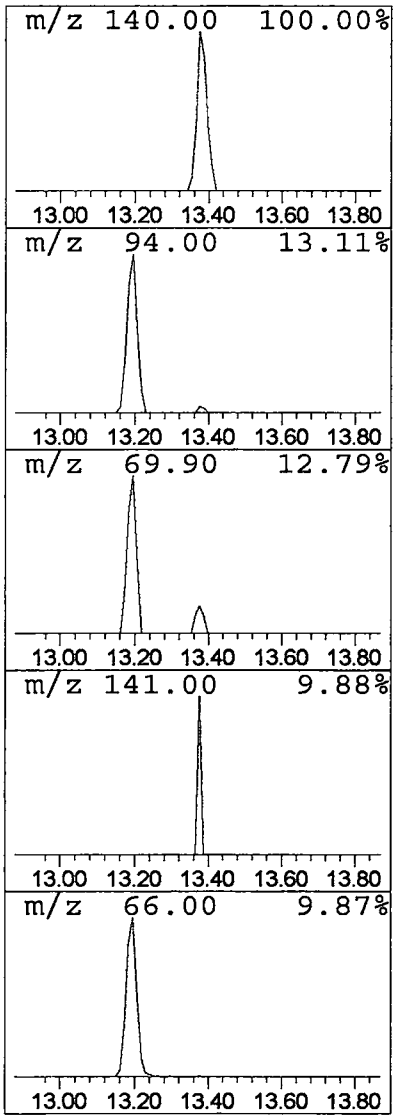
Peak Number 6 2-Methoxy-3-hydrazinyl-pyra... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	0.06 ug/L	39172	Naphthalene-d8	13.19

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxy-3-hydrazinyl-pyrazine	140	C5H8N4O	000000-00-0	78
2	4H-Pyran-4-one, 2-ethyl-3-hydrox...	140	C7H8O3	004940-11-8	56
3	Pyridine, 4-nitro-, 1-oxide (CAS...	140	C5H4N2O3	001124-33-0	50
4	Pyrimidinetetramine- $$ Pyrimidi...	140	C4H8N6	001004-74-6	39





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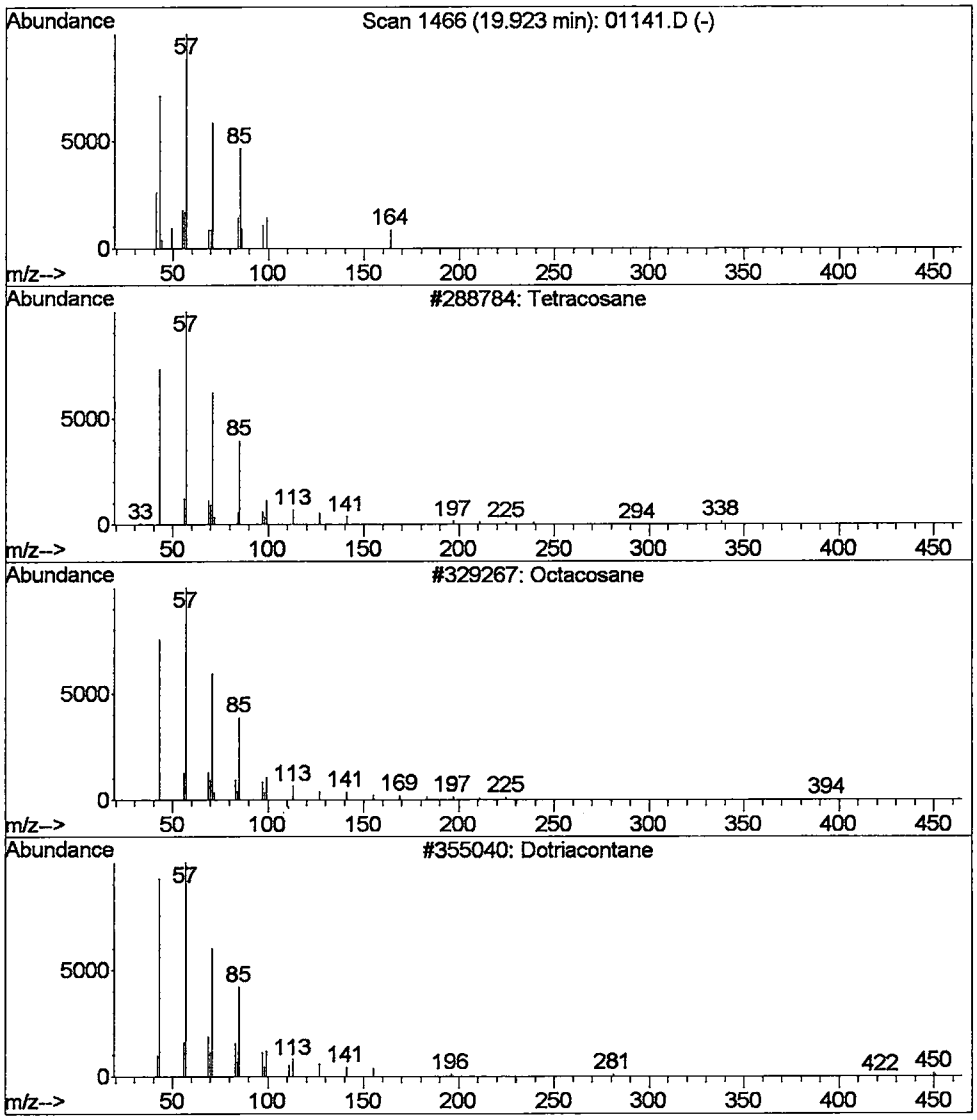
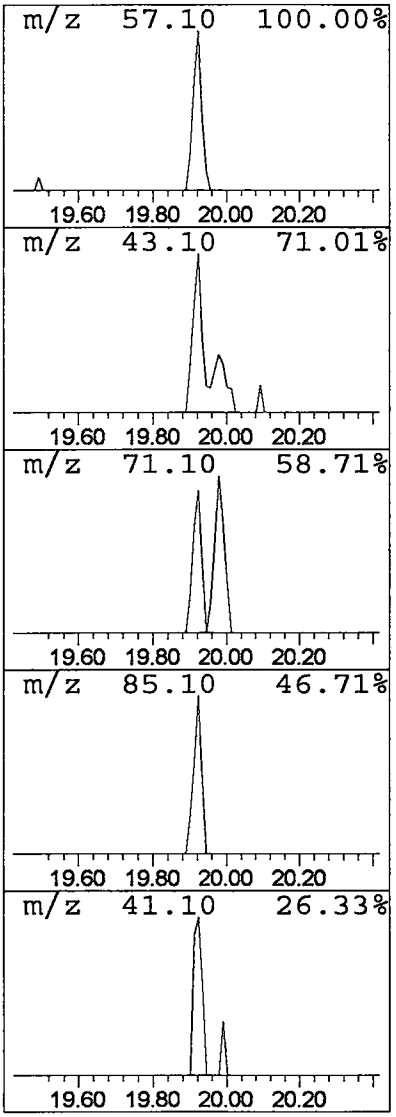
****

Peak Number 7 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	0.07 ug/L	46412	Acenaphthene-d10	18.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	64
2	Octacosane	394	C28H58	000630-02-4	64
3	Dotriacontane	451	C32H66	000544-85-4	64
4	Pentatriacontane	493	C35H72	000630-07-9	64





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Misc : February 25, 2002 Multiplr: 1.00
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Library : C:\DATABASE\WILEY7N.L

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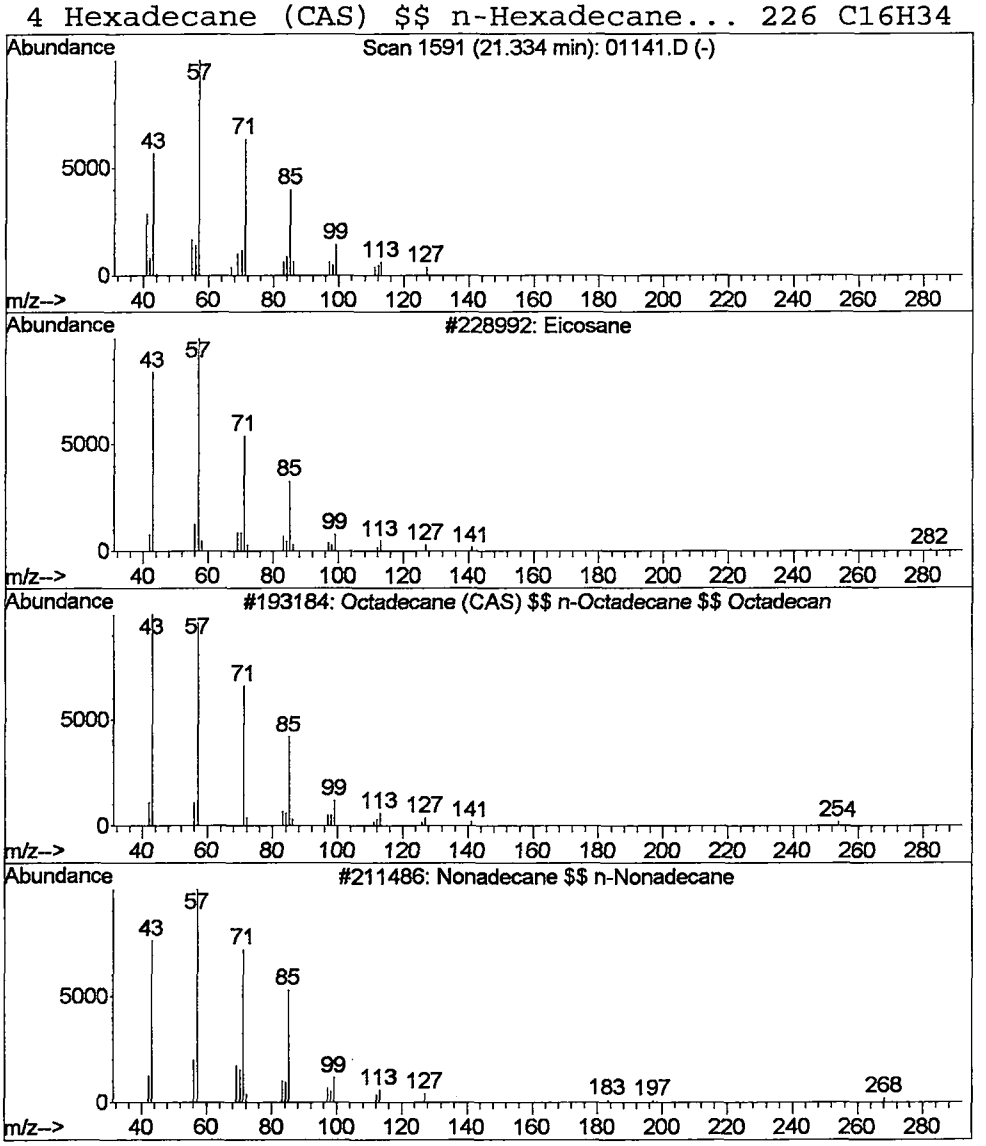
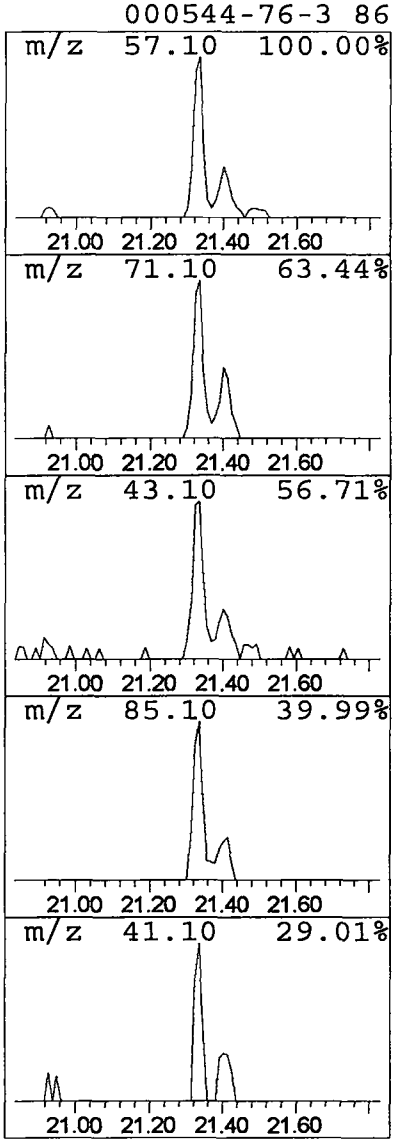
Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.33	0.15 ug/L	106215	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octadecane (CAS) $$ n-Octadecane...	254	C18H38	000593-45-3	90
3	Nonadecane $$ n-Nonadecane	268	C19H40	000629-92-5	87
4	Hexadecane (CAS) $$ n-Hexadecane...	226	C16H34	000544-76-3	86





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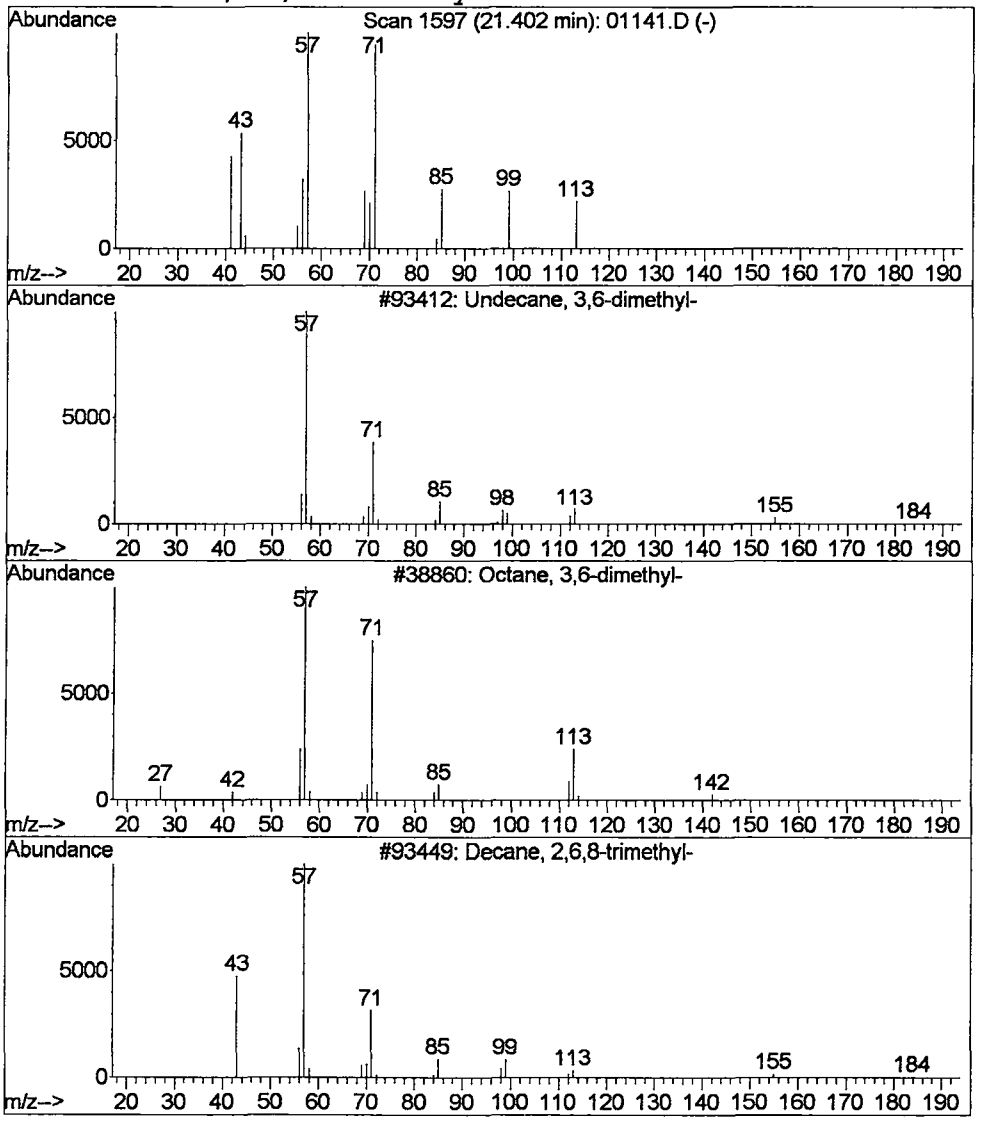
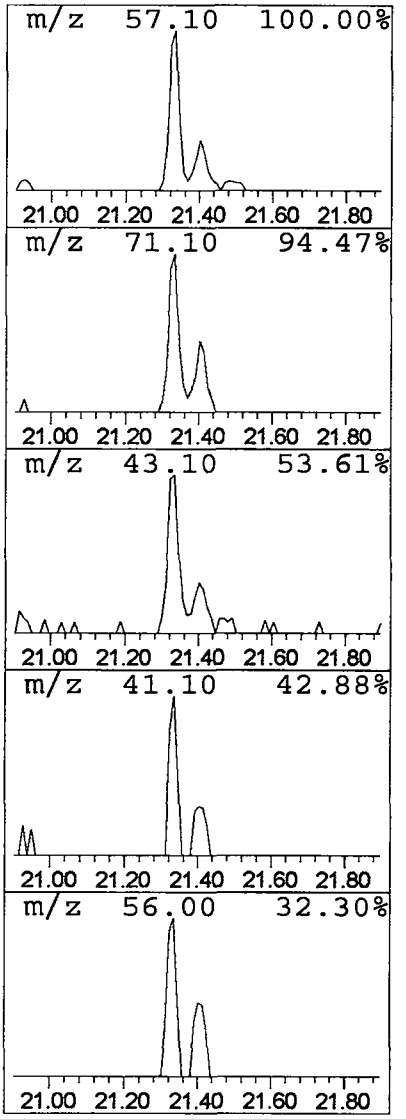
Peak Number 9 Undecane, 3,6-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	0.06 ug/L	38789	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	64
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	45
3	Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	42
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	40





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Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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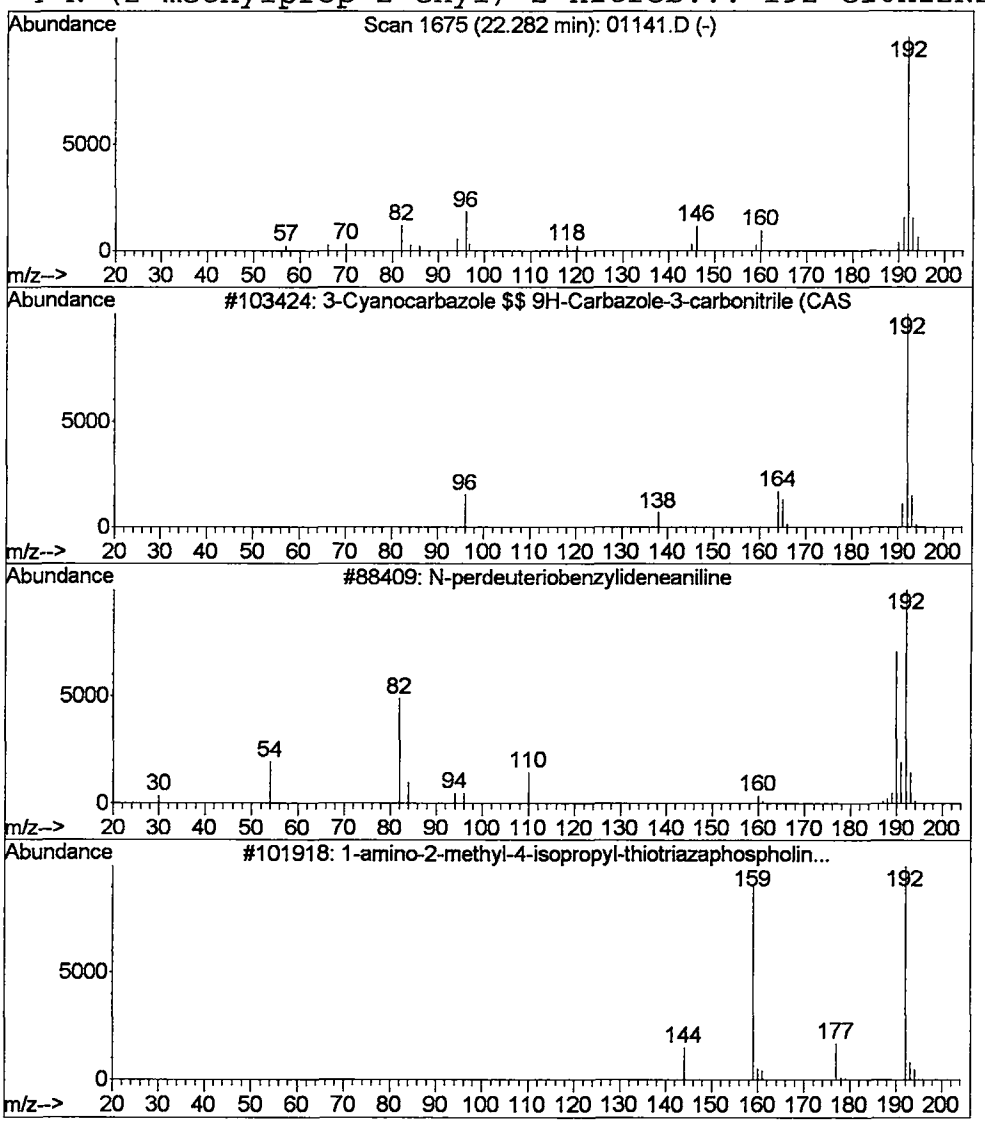
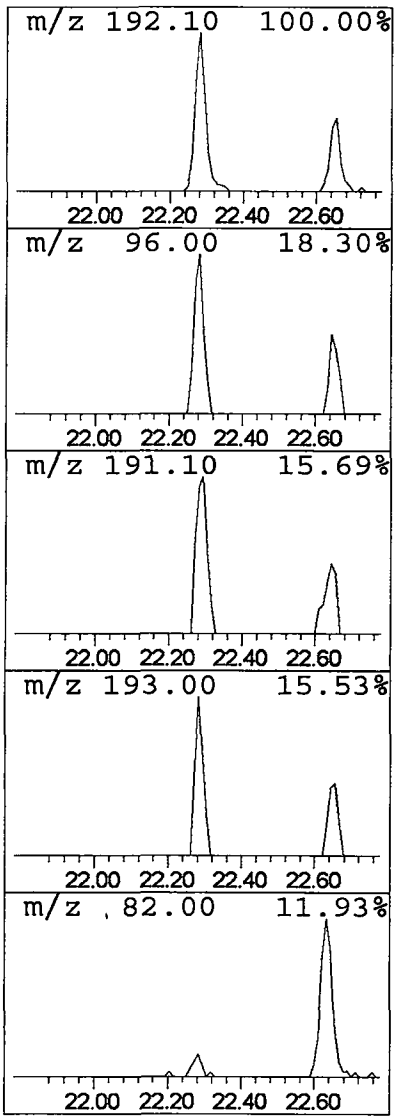
Peak Number 10 3-Cyanocarbazole $$ 9H-Carb... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.28	0.13 ug/L	88340	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyanocarbazole $$ 9H-Carbazole...	192	C13H8N2	057102-93-9	59
2	N-perdeuteriobenzylideneaniline	192	C13D11N	000538-51-2	58
3	1-amino-2-methyl-4-isopropyl-thi...	192	C5H13N4PS	107264-54-0	50
4	N-(2-methylprop-2-enyl)-2-nitrob...	192	C10H12N2O2	000000-00-0	47





Data File : C:\MSDCHEM\1\5973N\02FEB25\01141.D Vial: 7
Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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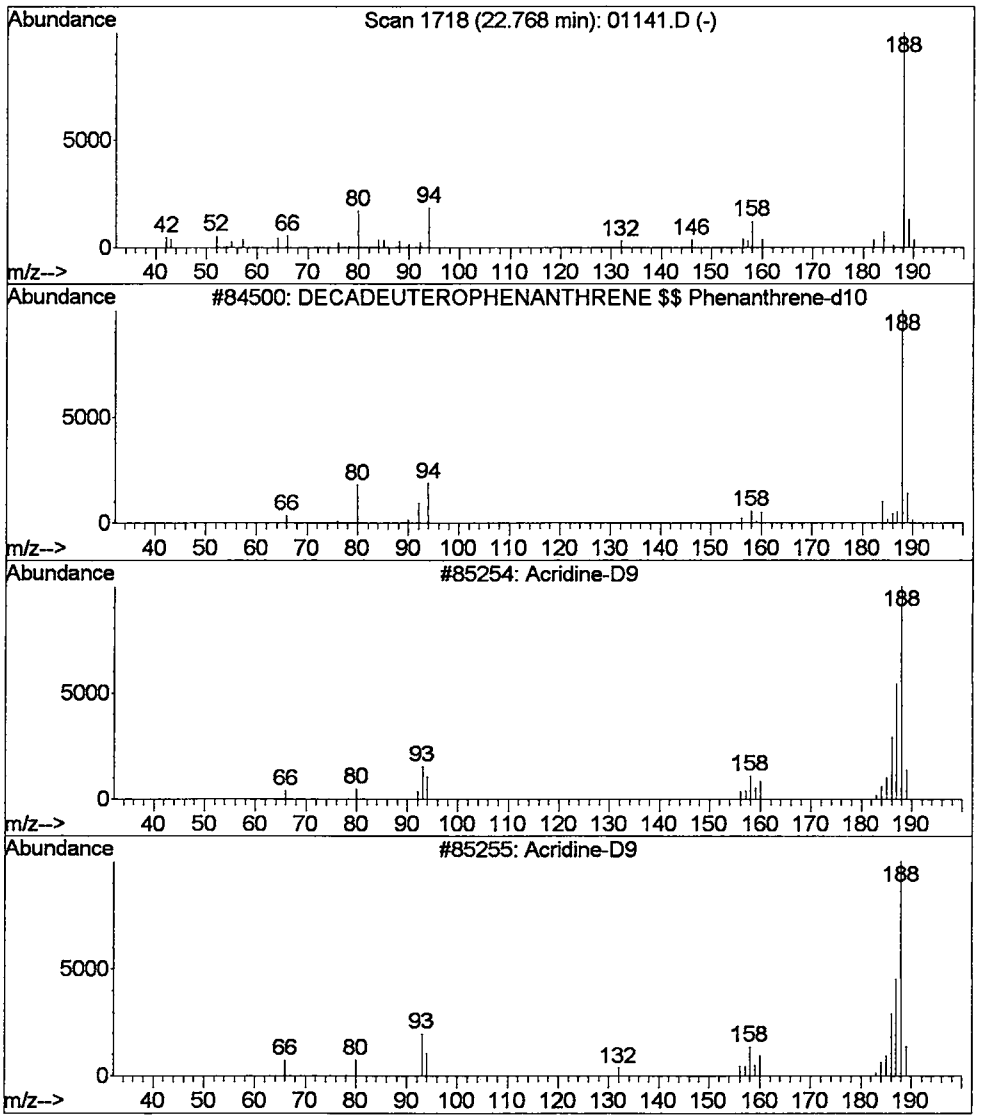
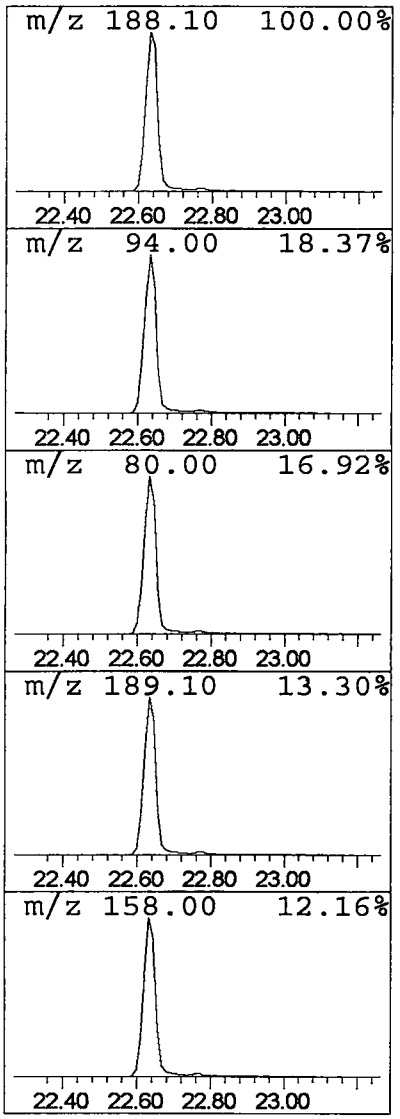
Peak Number 11 DECADEUTEROPHENANTHRENE $$ ... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.77	0.58 ug/L	403812	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	DECADEUTEROPHENANTHRENE $$ Phena...	188	C14D10	001517-22-2	83
2	Acridine-D9	188	C13D9N	000000-00-0	80
3	Acridine-D9	188	C13D9N	000000-00-0	80
4	Anthracene-d10-	188	C14D10	001719-06-8	78





Data File : C:\MSDCHEM\1\5973N\02FEB25\01141.D Vial: 7
Acq On : 25 Feb 2002 4:11 pm Operator:
Sample : 508 scan Inst : Instrumen
Misc : February 25, 2002 Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title : 508 scan method
Library : C:\DATABASE\WILEY7N.L

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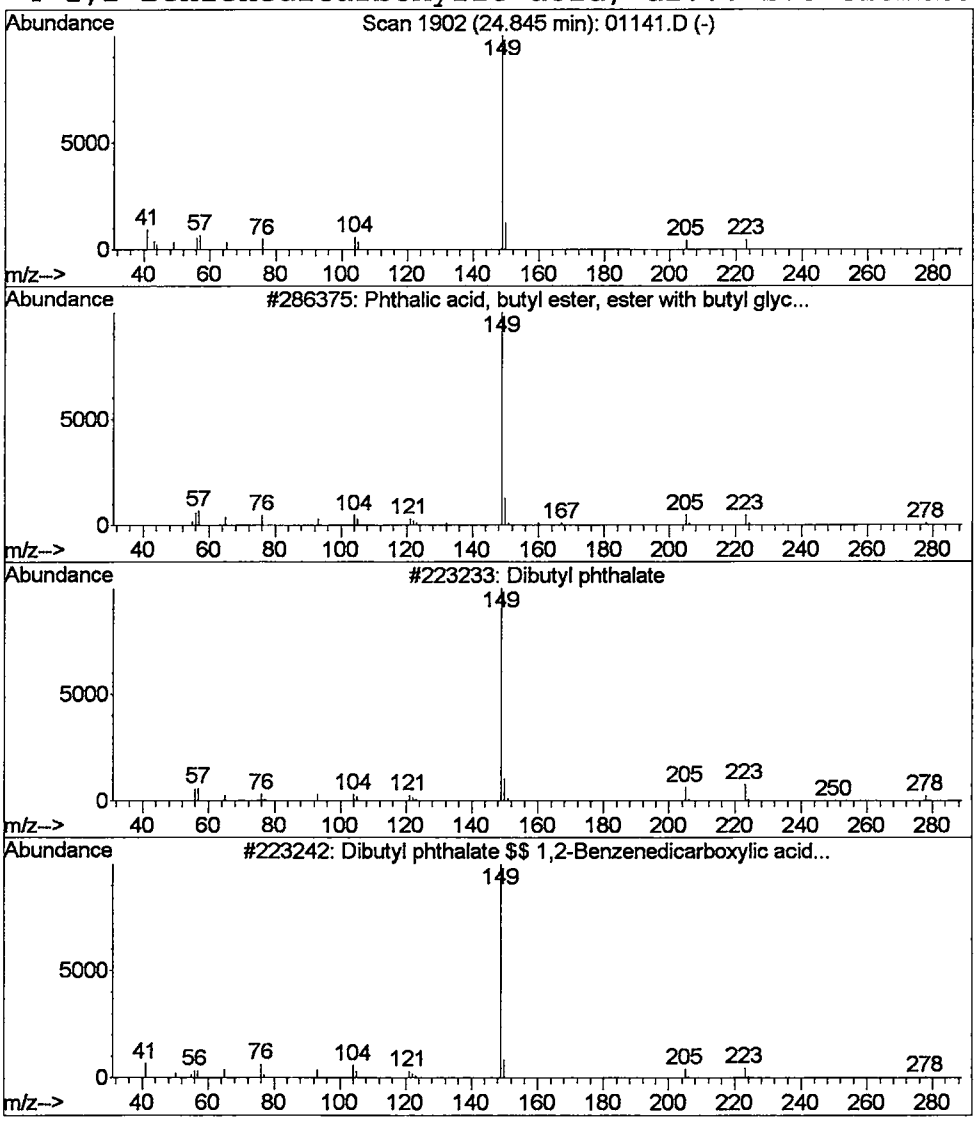
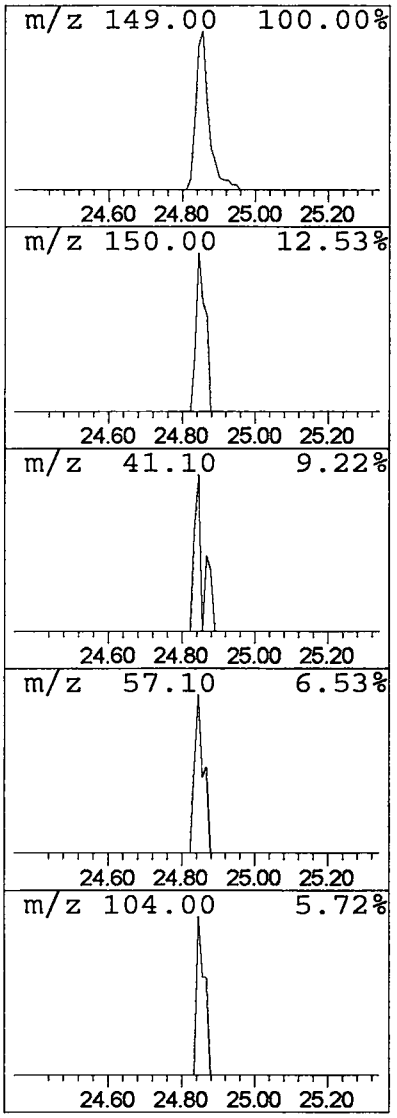
Peak Number 12 Phthalic acid, butyl ester,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.84	0.09 ug/L	66372	Phenanthrene-d10	22.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phthalic acid, butyl ester, este...	336	C18H24O6	000085-70-1	83
2	Dibutyl phthalate	278	C16H22O4	000084-74-2	83
3	Dibutyl phthalate $$ 1,2-Benzene...	278	C16H22O4	000084-74-2	83
4	1,2-Benzenedicarboxylic acid, di...	278	C16H22O4	000084-74-2	83





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Data File : C:\MSDCHEM\1\5973N\02FEB25\01141.D          Vial: 7
Acq On    : 25 Feb 2002   4:11 pm                    Operator:
Sample    : 508 scan                                 Inst    : Instrumen
Misc      : February 25, 2002                        Multiplr: 1.00
MS Integration Params: LSCINT.P

Quant Method : C:\MSDCHEM\1...\HP022102.M (RTE Integrator)
Title        : 508 scan method
Library      : C:\DATABASE\WILEY7N.L
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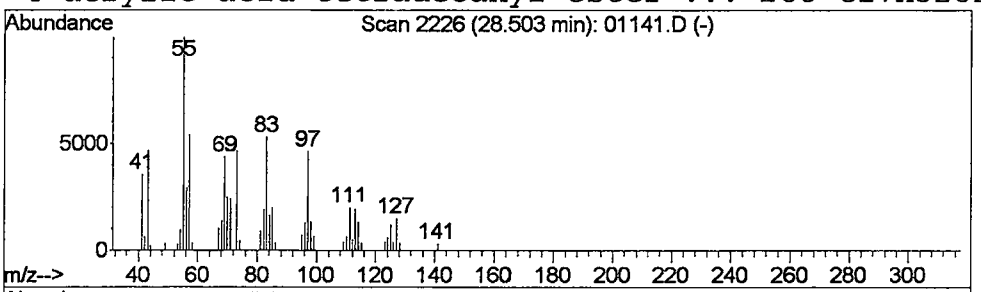
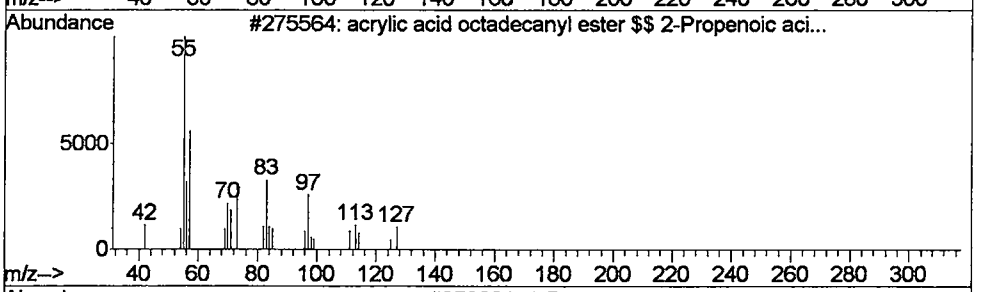
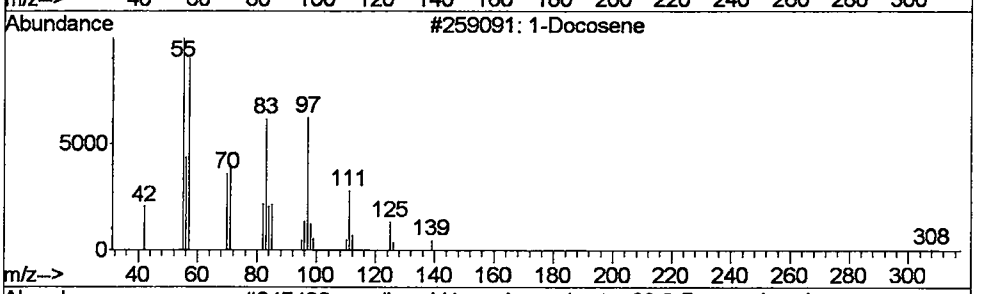
Peak Number 13 acrylic acid octadecanyl es... Concentration Rank 2

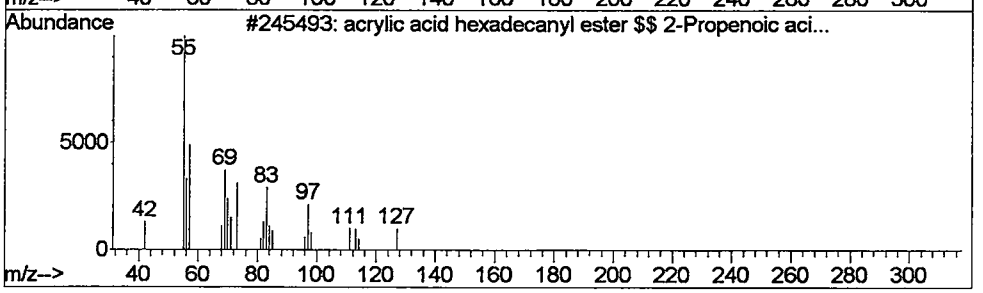
R.T.	EstConc	Area	Relative to ISTD	R.T.
28.50	0.44 ug/L	273811	Chrysene-d12	30.49

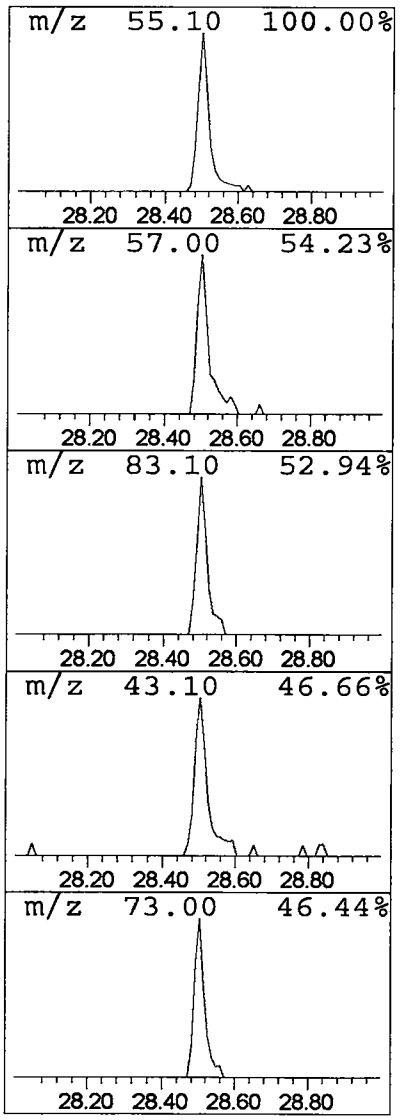
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	acrylic acid octadecanyl ester $...	324	C21H40O2	004813-57-4	90
2	1-Docosene	308	C22H44	001599-67-3	70
3	acrylic acid hexadecanyl ester $...	296	C19H36O2	013402-02-3	68
4	acrylic acid tetradecanyl ester ...	268	C17H32O2	021643-42-5	64











Operator ID: Date Acquired: 25 Feb 2002 4:11 pm
Data File: C:\MSDCHEM\1\5973N\02FEB25\01141.D
Name: 508 scan
Misc: February 25, 2002
Method: C:\MSDCHEM\1\METHODS\METHODS\HP022102.M (RTE Integrator)
Title: 508 scan method
Library Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
Acetonitrile, dic...	3.50	0.1	ug/L	53929	1	9.72	8356120	20.0
Butanoic acid, me...	3.62	0.2	ug/L	66250	1	9.72	8356120	20.0
3-(CYCLOHEX-3'-EN...	5.95	0.3	ug/L	138149	1	9.72	8356120	20.0
2-Propanone, 1,1,...	6.00	0.3	ug/L	127618	1	9.72	8356120	20.0
Cyclopentasiloxan...	12.54	0.4	ug/L	227463	2	13.19	12372700	20.0
2-Methoxy-3-hydra...	13.38	0.1	ug/L	39172	2	13.19	12372700	20.0
Tetracosane	19.92	0.1	ug/L	46412	3	18.33	13374400	20.0
Eicosane	21.33	0.2	ug/L	106215	4	22.63	14014800	20.0
Undecane, 3,6-dim...	21.40	0.1	ug/L	38789	4	22.63	14014800	20.0
3-Cyanocarbazole ...	22.28	0.1	ug/L	88340	4	22.63	14014800	20.0
DECADEUTEROPHENAN...	22.77	0.6	ug/L	403812	4	22.63	14014800	20.0
Phthalic acid, bu...	24.84	0.1	ug/L	66372	4	22.63	14014800	20.0
acrylic acid octa...	28.50	0.4	ug/L	273811	5	30.49	12419300	20.0