Comments for Sample AE10206 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 05-21-2002 Time: 12:07:20

The GCMS scan, from 35 to 550 amu, does not reveal the presence of unusual compounds.
The recovery for 1 of the 43 compounds in the LCS Standard was low. This sample will be re-extracted because of the low Surrogate Standard recovery.
Re-analysis yielded a Surrogate Standard recovery of 89%.

User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 05/21/2002 Time: 12:06:53

Sample: AE10206
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 5/10/02 12:07 Ended: 5/10/02 12:07 Analyst: DLV
Result source: manual entry
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Sum 2,4 DDD	LSPEC	62		10.0

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
Sample : 5/10 eh Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: EVENTS.E
Quant Time: May 17 09:44:30 2002 Quant Results File: 050102.RES

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Last Update : Mon May 13 11:40:29 2002
Response via : Initial Calibration
DataAcq Meth : 508SCAN

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.94	152	5572970	40.00	ug/L	0.00
10) Napthalene-d8	13.43	136	22171094	40.00	ug/L	0.00
17) Acenapthalene-d10	18.57	164	12091246	40.00	ug/L	0.00
29) Phenanthranene-d10	22.95	188	17592939	40.00	ug/L	0.00
37) Chrysene-d12	30.81	240	12694887	40.00	ug/L	0.00
43) Perylene-d12	34.70	264	7876864	40.00	ug/L	0.00
System Monitoring Compounds						
27) TCMX	20.55	209	2611328	35.57	ug/L	0.00
Spiked Amount 40.000			Recovery =	88.92%		
Target Compounds						Qvalue
2) n-nitros-dimethyl amine	0.00	74	0	N.D.	d	
3) bis(2-Chloroethyl)ether	0.00	93	0	N.D.		
4) 1,3-Dichlorobenzene	0.00	146	0	N.D.		
5) 1,4-Dichlorobenzene	0.00	146	0	N.D.		
6) 1,2-Dichlorobenzene	0.00	146	0	N.D.		
7) 2,2'oxybis(1-Chloropropane	0.00	45	0	N.D.		
8) N-nitroso-di-propylamine	0.00	70	0	N.D.		
9) Hexachloroethane	0.00	117	0	N.D.		
11) Nitrobenzene	0.00	77	0	N.D.		
12) Isophorone	0.00	82	0	N.D.		
13) bis(2-Chloroethoxy) methan	0.00	93	0	N.D.		
14) 1,2,4-Trichlorobenzene	0.00	180	0	N.D.		
15) Napthalene	0.00	128	0	N.D.		
16) Hexachlorobutadiene	0.00	225	0	N.D.		
18) 2-Chloronaphthalene	0.00	162	0	N.D.		
19) Dimethylphthalate	0.00	163	0	N.D.		
20) 2,6-Dinitrotoluene	0.00	165	0	N.D.		
21) Acenapthylene	0.00	152	0	N.D.		
22) Acenapthalene	0.00	153	0	N.D.		
23) 2,4-Dinitrotoluene	0.00	165	0	N.D.		
24) Diethylphthalate	0.00	149	0	N.D.		
25) 4-Chlorophenyl-phenylether	0.00	204	0	N.D.		
26) Fluorene	0.00	166	0	N.D.		
28) Azobenzene	20.54	77	44710	N.D.		
30) Nnitrosodiphenylamine	20.54	169	48057	N.D.		
31) 4-Bromophenyl-phenylether	0.00	248	0	N.D.		
32) Hexachlorobenzene	0.00	284	0	N.D.		
33) Phenanthrene	0.00	178	0	N.D.		
34) Anthracene	0.00	178	0	N.D.		
35) Di-n-butylphthalate	25.09	149	21636	N.D.		

(#) = qualifier out of range (m) = manual integration

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Acq On : 16 May 2002 7:25 pm Operator: Mclean
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Misc : Multiplr: 1.00
MS Integration Params: EVENTS.E
Quant Time: May 17 09:44:30 2002 Quant Results File: 050102.RES

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Last Update : Mon May 13 11:40:29 2002
Response via : Initial Calibration
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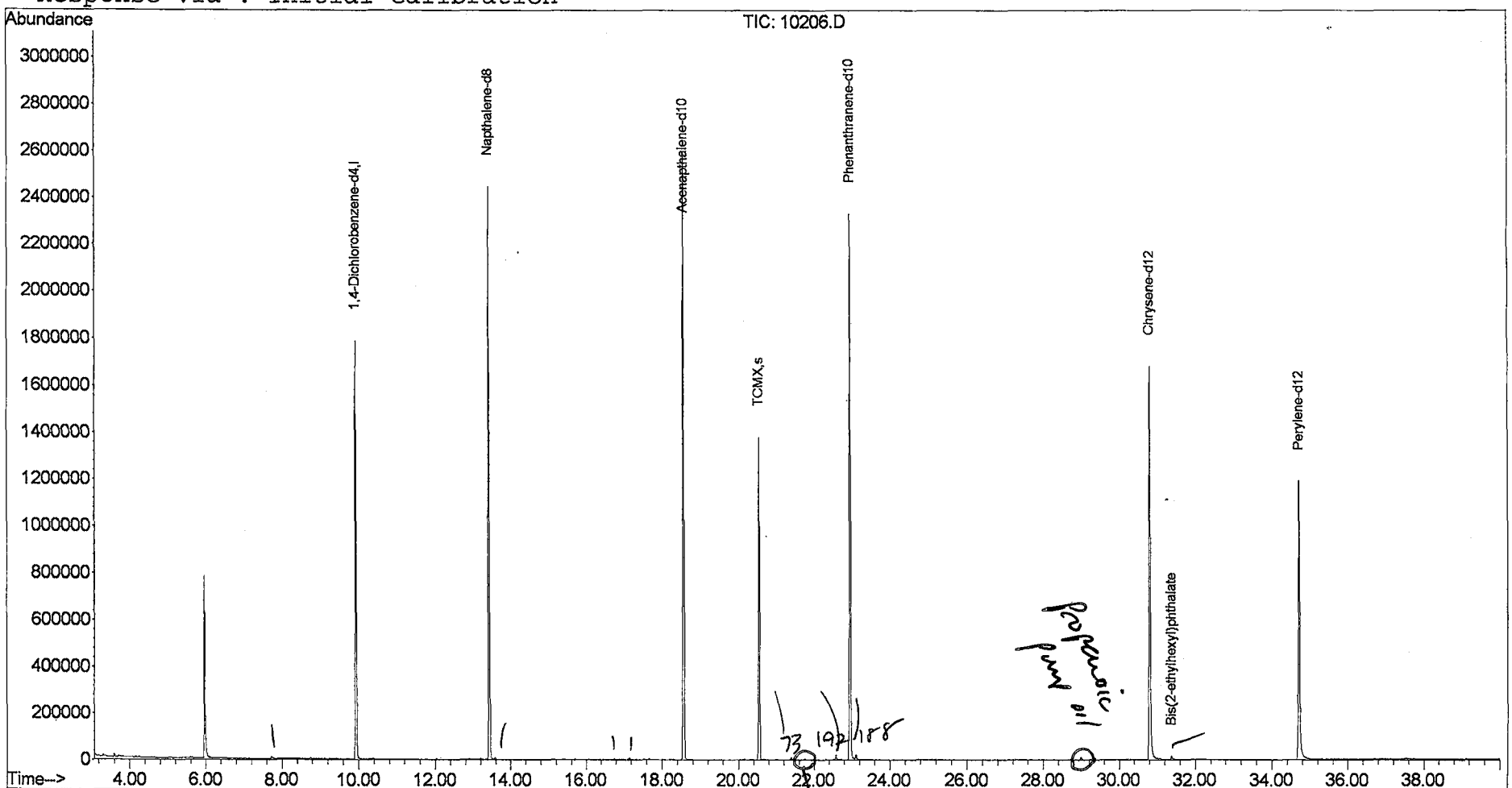
	Compound	R.T.	QIon	Response	Conc Unit	Qvalue
36)	Fluoroanthene	0.00	202	0	N.D.	
38)	Pyrene	0.00	202	0	N.D.	
39)	Butylbenzylphthalate	0.00	149	0	N.D.	
40)	Benzo(a)anthracene	30.80	228	32765	N.D.	
41)	Bis(2-ethylhexyl)phthalate	31.38	149	100337	0.32 ug/L #	91
42)	Chrysene	0.00	228	0	N.D.	
44)	Di-n-octylphthalate	0.00	149	0	N.D.	
45)	Benzo(b)fluoranthene	0.00	252	0	N.D.	
46)	Benzo(k)fluoranthene	0.00	252	0	N.D.	
47)	Benzo(a)pyrene	0.00	252	0	N.D.	
48)	Indeno(1,2,3-cd)pyrene	0.00	276	0	N.D.	
49)	Dibenz(a,h)anthracene	0.00	278	0	N.D.	
50)	Benzo(g,h,i)perylene	0.00	276	0	N.D.	

(#) = qualifier out of range (m) = manual integration (+) = signals summed

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
Sample : 5/10 eh Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: EVENTS.E
Quant Time: May 17 15:02 2002 Quant Results File: 050102.RES

Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Last Update : Mon May 13 11:40:29 2002
Response via : Initial Calibration



Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
Sample : 5/10 eh Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.e

Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan

Signal : TIC

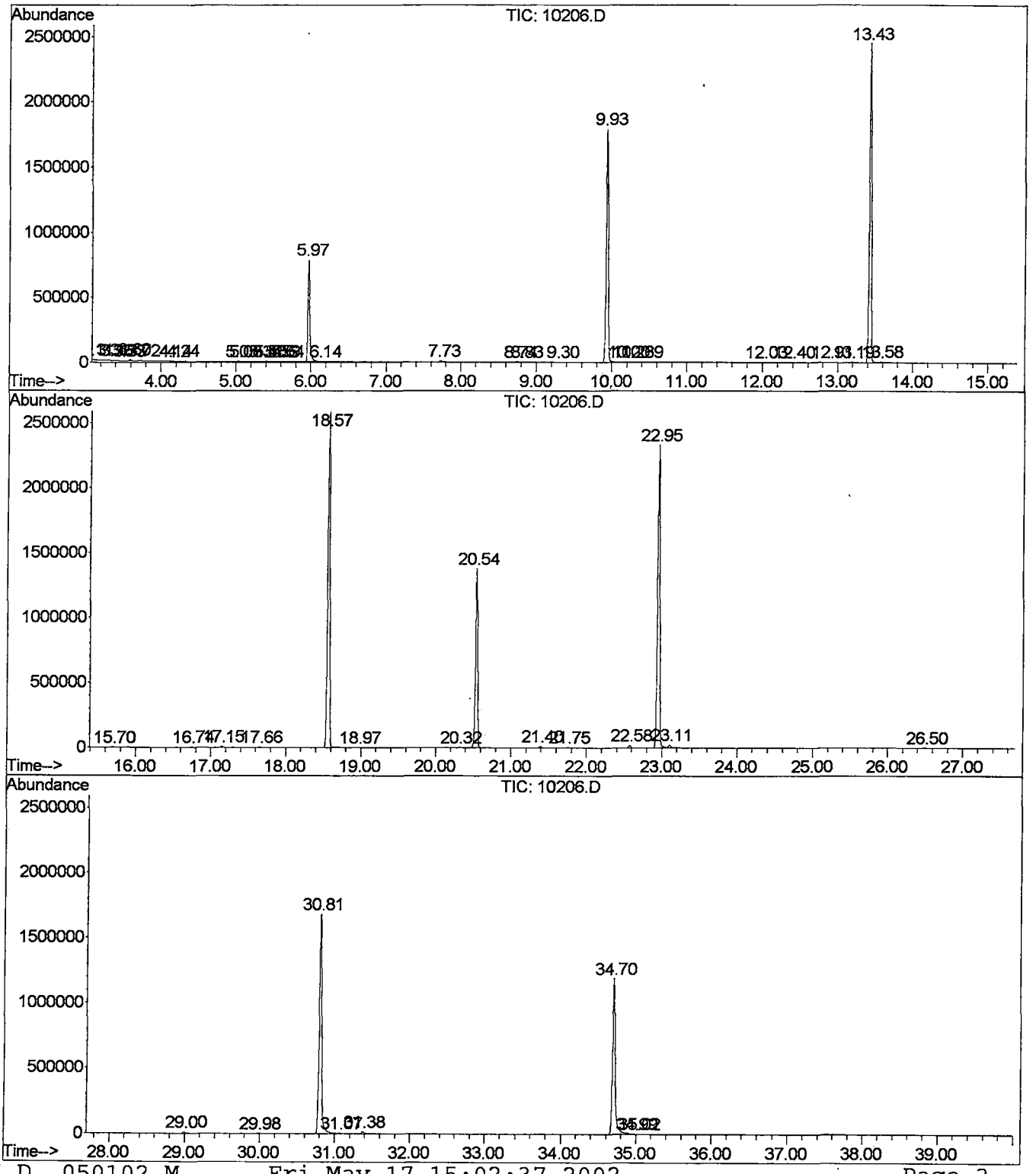
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.109	3	5	14	BV 4	2820	33002	0.07%	0.011%
2	3.308	35	39	44	PV 4	6048	76620	0.15%	0.026%
3	3.361	44	48	74	VV 4	3226	88813	0.18%	0.031%
4	3.526	74	76	80	PV 4	1917	25154	0.05%	0.009%
5	3.596	83	88	94	VV	12985	221266	0.44%	0.076%
6	3.726	101	110	124	VV 2	7004	276938	0.56%	0.095%
7	4.143	176	181	194	VV 7	3012	93472	0.19%	0.032%
8	4.243	194	198	203	VV 4	3007	50324	0.10%	0.017%
9	5.030	325	332	337	PV 7	3402	83962	0.17%	0.029%
10	5.077	337	340	350	VV 9	3407	97566	0.20%	0.034%
11	5.341	378	385	390	VV 7	2157	58045	0.12%	0.020%
12	5.406	390	396	401	VV 5	4204	107420	0.22%	0.037%
13	5.559	418	422	424	PV 4	1698	21089	0.04%	0.007%
14	5.594	424	428	430	VV 3	2079	35114	0.07%	0.012%
15	5.635	430	435	444	VV 5	3123	83428	0.17%	0.029%
16	5.970	484	492	519	VV	787791	14350368	28.77%	4.943%
17	6.140	519	521	526	VV 5	3029	47189	0.09%	0.016%
18	7.727	786	791	804	PV 3	8510	211281	0.42%	0.073%
19	8.743	959	964	973	VV 3	3606	77288	0.15%	0.027%
20	8.826	973	978	984	PV 5	1669	30407	0.06%	0.010%
21	9.301	1055	1059	1069	PV 4	1967	41614	0.08%	0.014%
22	9.936	1158	1167	1184	VV	1770479	33579353	67.33%	11.568%
23	10.200	1206	1212	1218	VV 6	2383	36670	0.07%	0.013%
24	10.259	1218	1222	1232	PV 6	2910	62098	0.12%	0.021%
25	10.388	1235	1244	1247	PV 7	1397	25690	0.05%	0.009%
26	12.034	1520	1524	1530	VV 2	2650	46068	0.09%	0.016%
27	12.404	1576	1587	1593	BV 5	2281	38908	0.08%	0.013%
28	12.909	1662	1673	1679	PV 6	2746	73942	0.15%	0.025%
29	13.197	1716	1722	1729	BV 2	4916	89047	0.18%	0.031%
30	13.432	1752	1762	1783	PV	2419711	45224292	90.67%	15.579%
31	13.579	1783	1787	1793	VV	6863	112850	0.23%	0.039%
32	15.700	2140	2148	2155	PV 3	2201	37909	0.08%	0.013%
33	16.746	2321	2326	2332	PV 4	3692	65297	0.13%	0.022%
34	17.151	2382	2395	2402	PV 6	9044	145035	0.29%	0.050%
35	17.657	2472	2481	2486	BV 3	3881	56116	0.11%	0.019%
36	18.567	2625	2636	2654	PV	2558871	49876177	100.00%	17.182%
37	18.967	2695	2704	2709	VV 2	1677	40224	0.08%	0.014%

39	20.547	2960	2973	2991	PV	1358519	25959616	52.05%	8.943%
40	21.393	3104	3117	3123	BV	3 11768	192902	0.39%	0.066%
41	21.758	3168	3179	3186	PV	5 4472	74758	0.15%	0.026%
42	22.580	3308	3319	3331	VV	2 20281	357129	0.72%	0.123%
43	22.950	3363	3382	3402	PV	2 2294794	48031108	96.30%	16.546%
44	23.109	3402	3409	3416	VV	2 19448	437602	0.88%	0.151%
45	26.505	3978	3987	3993	VV	3 2125	44536	0.09%	0.015%
46	28.996	4390	4411	4417	VV	5 11541	220311	0.44%	0.076%
47	29.984	4572	4579	4584	PV	4 1961	42343	0.08%	0.015%
48	30.806	4708	4719	4756	VV	2 1687280	39520804	79.24%	13.614%
49	31.065	4756	4763	4770	VV	7 4853	179768	0.36%	0.062%
50	31.376	4806	4816	4834	PV	2 14906	402322	0.81%	0.139%
51	34.702	5364	5382	5430	PV	2 1175951	29132261	58.41%	10.036%
52	34.995	5430	5432	5435	VV	3 1754	24304	0.05%	0.008%
53	35.025	5435	5437	5441	VV	4 1311	9986	0.02%	0.003%

Sum of corrected areas: 290287779

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\051602\10206.D
Operator : Mclean
Acquired : 16 May 2002 7:25 pm using AcqMethod 508SCAN
Instrument : Instrumen
Sample Name: 5/10 eh
Misc Info :
Vial Number: 7
Quant File :050102.RES (Chemstation Integrator)



Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
Sample : 5/10 eh Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.e

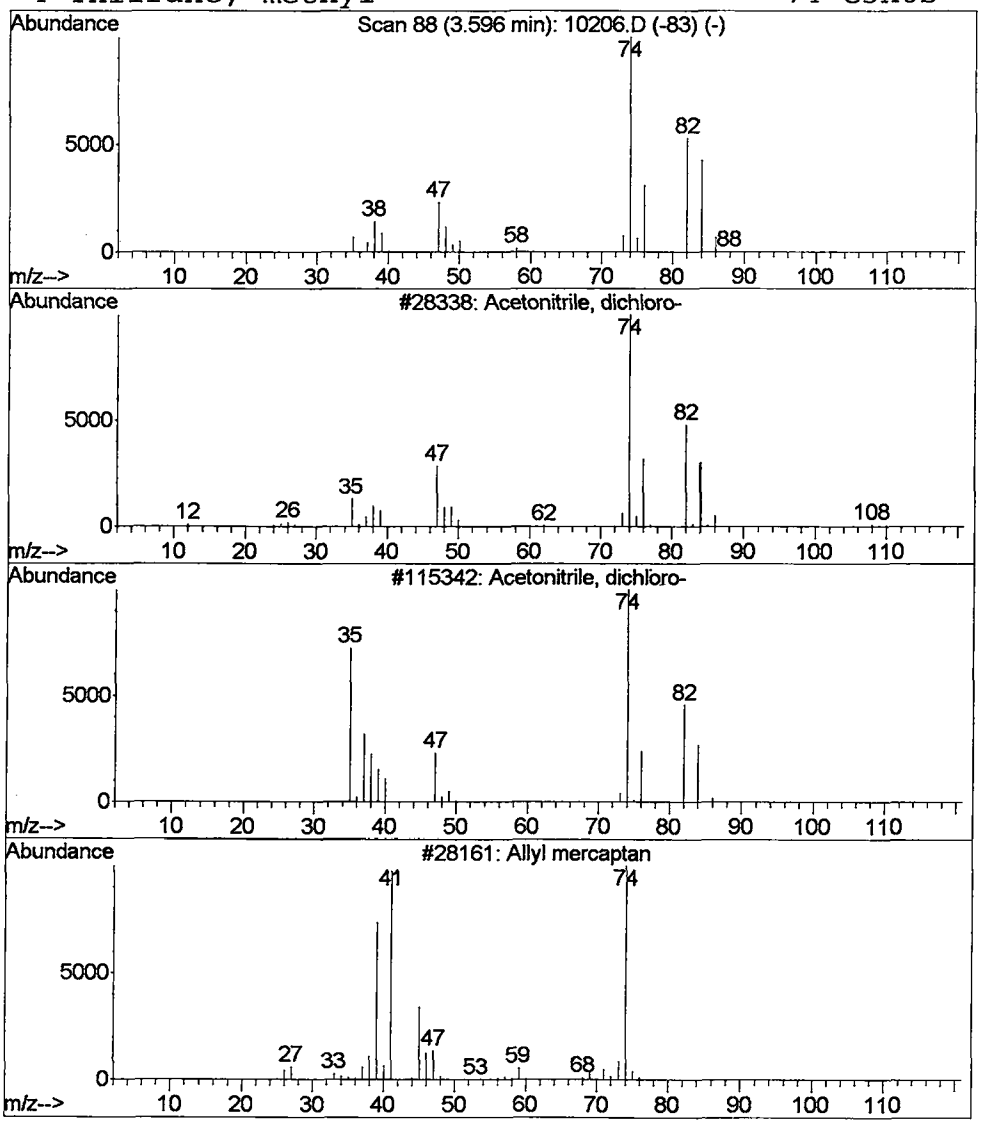
Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

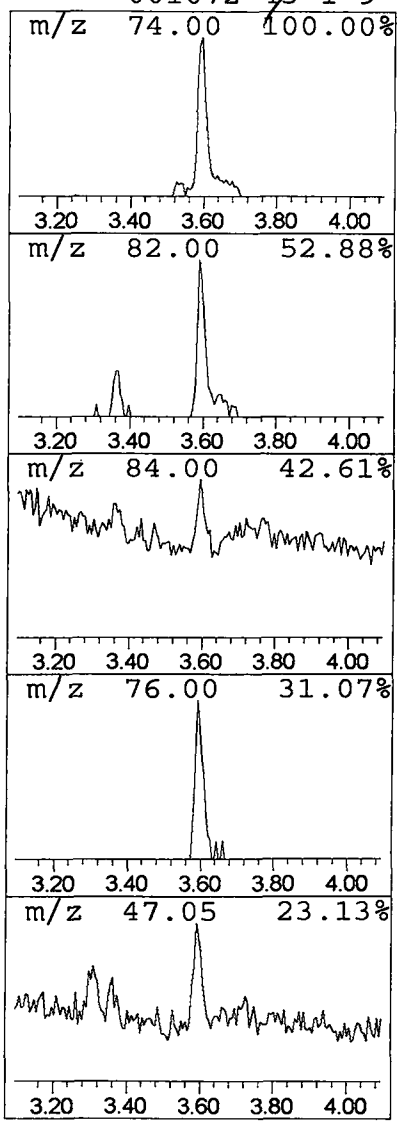
****

Peak Number 1 Acetonitrile, dichloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.60	0.26 ug/L	221266	1,4-Dichlorobenzene-d4	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	74
2	Acetonitrile, dichloro-	109	C2HCl2N	003018-12-0	39
3	Allyl mercaptan	74	C3H6S	000870-23-5	9
4	Thiirane, methyl-	74	C3H6S	001072-43-1	9





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Acq On : 16 May 2002 7:25 pm Operator: Mclean
Sample : 5/10 eh Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.e

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
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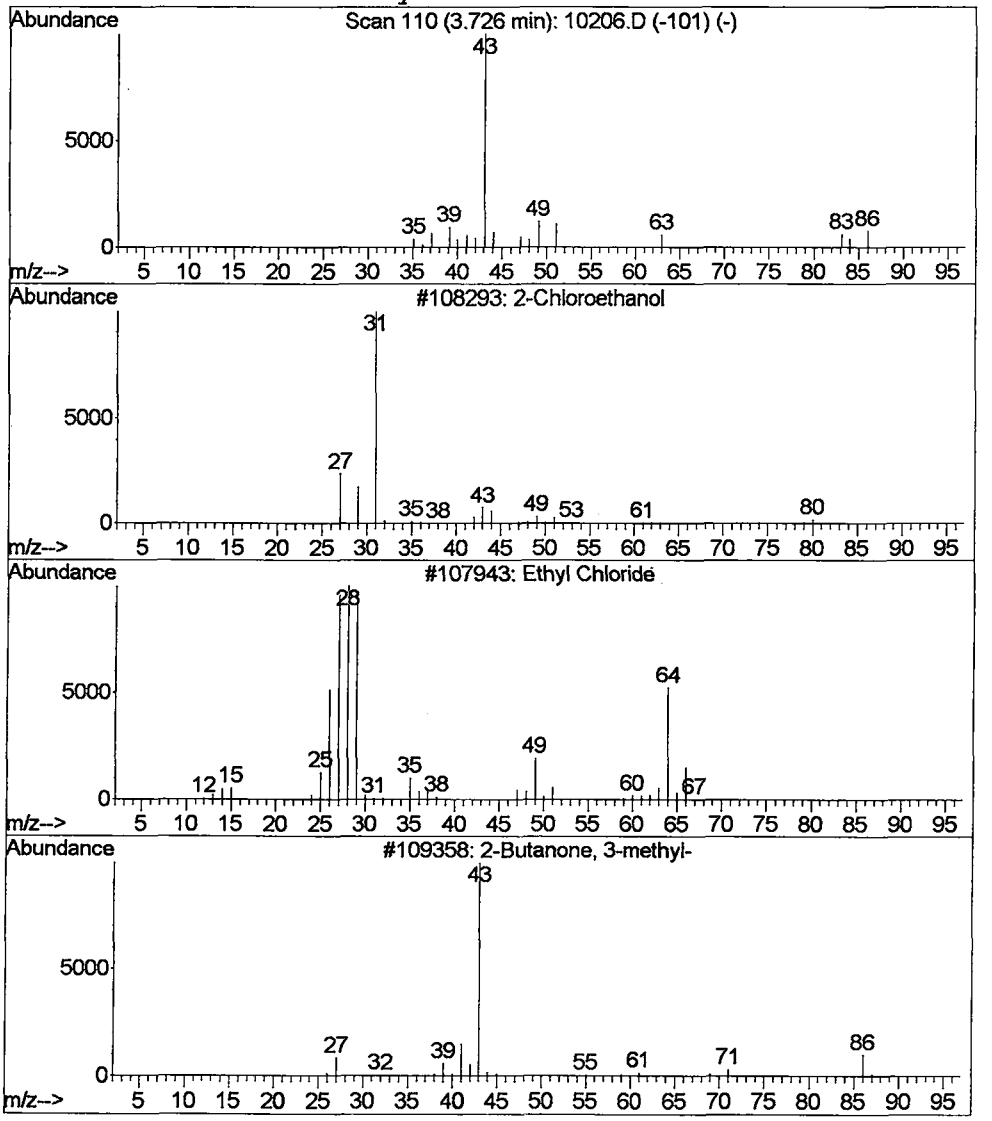
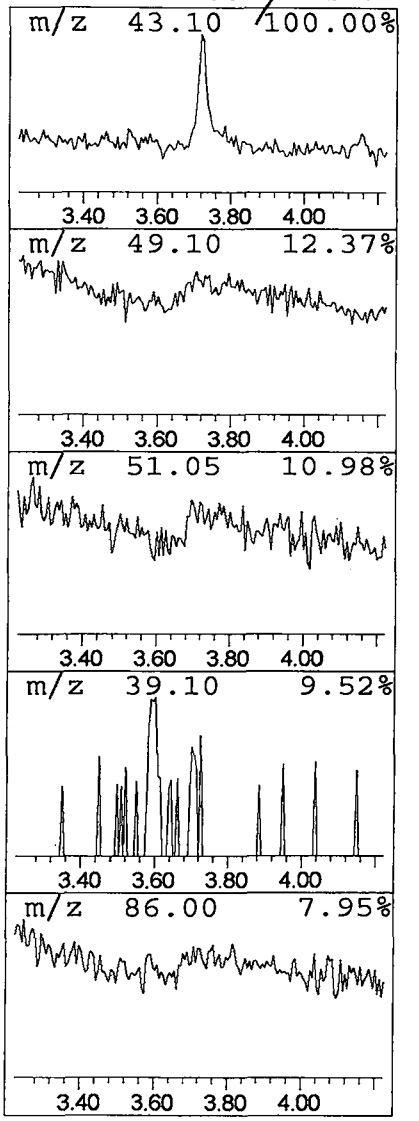
****

Peak Number 2 2-Chloroethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.72	0.33 ug/L	276938	1,4-Dichlorobenzene-d4	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Chloroethanol	80	C2H5ClO	000107-07-3	9
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	9
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	7
4	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	7





Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
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Library : C:\DATABASE\NIST98.L

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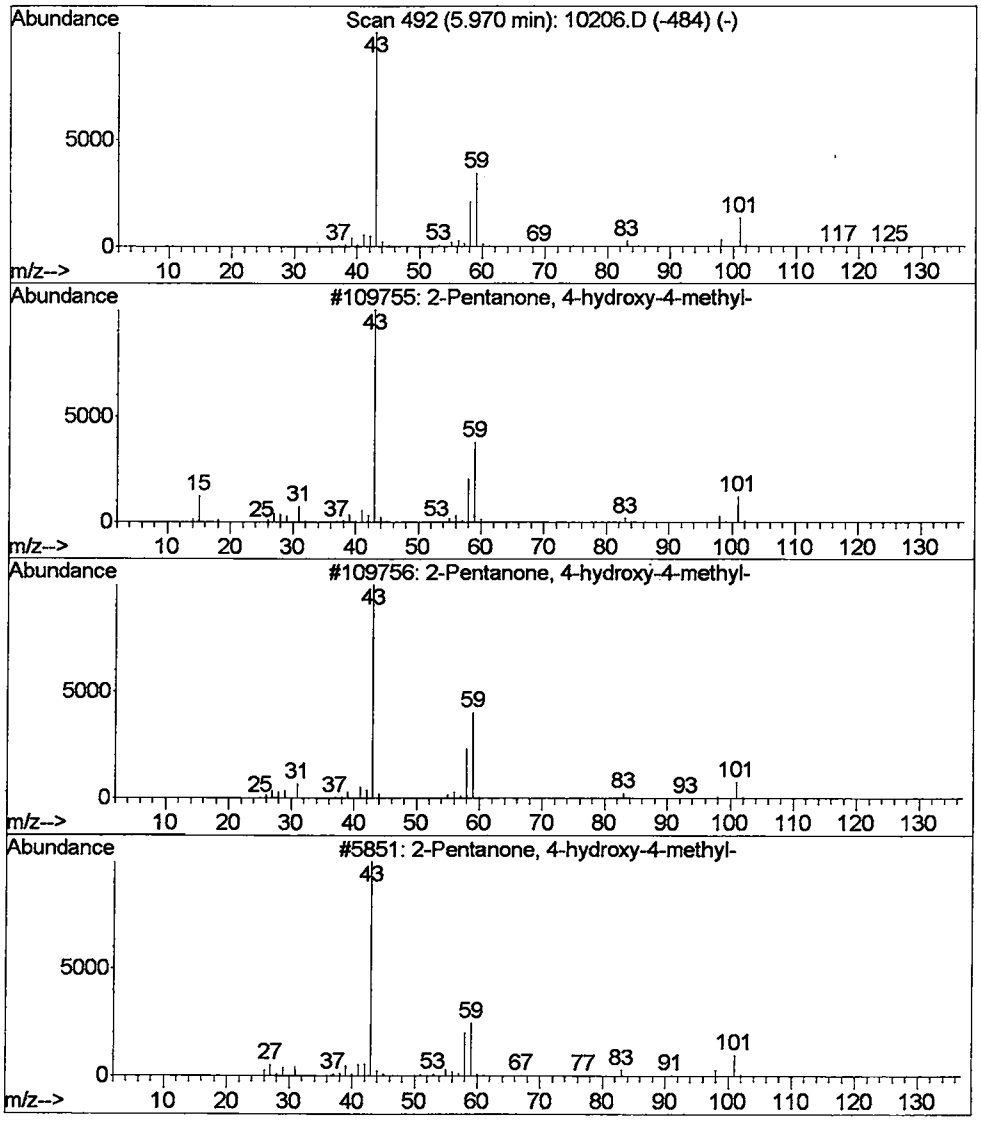
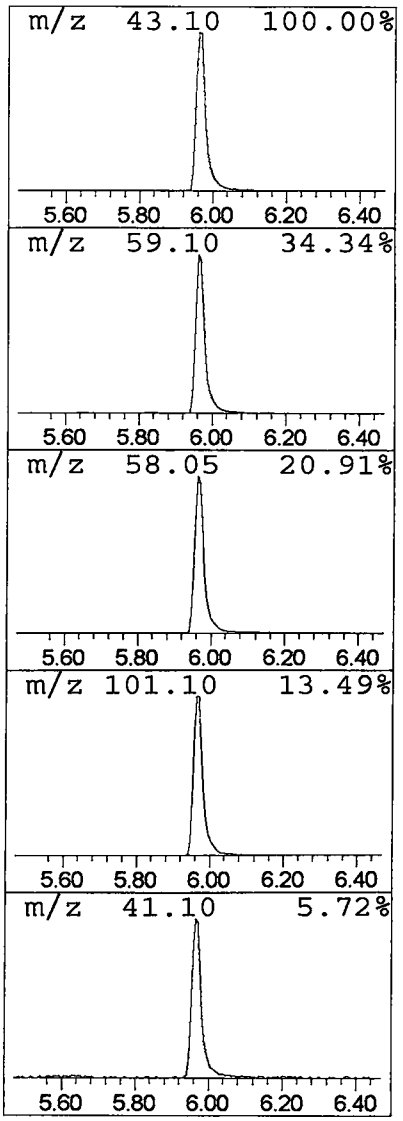
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.97	17.09 ug/L	14350400	1,4-Dichlorobenzene-d4	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	86
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
4	Acetone	58	C3H6O	000067-64-1	32





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MS Integration Params: LSCINT.e

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Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

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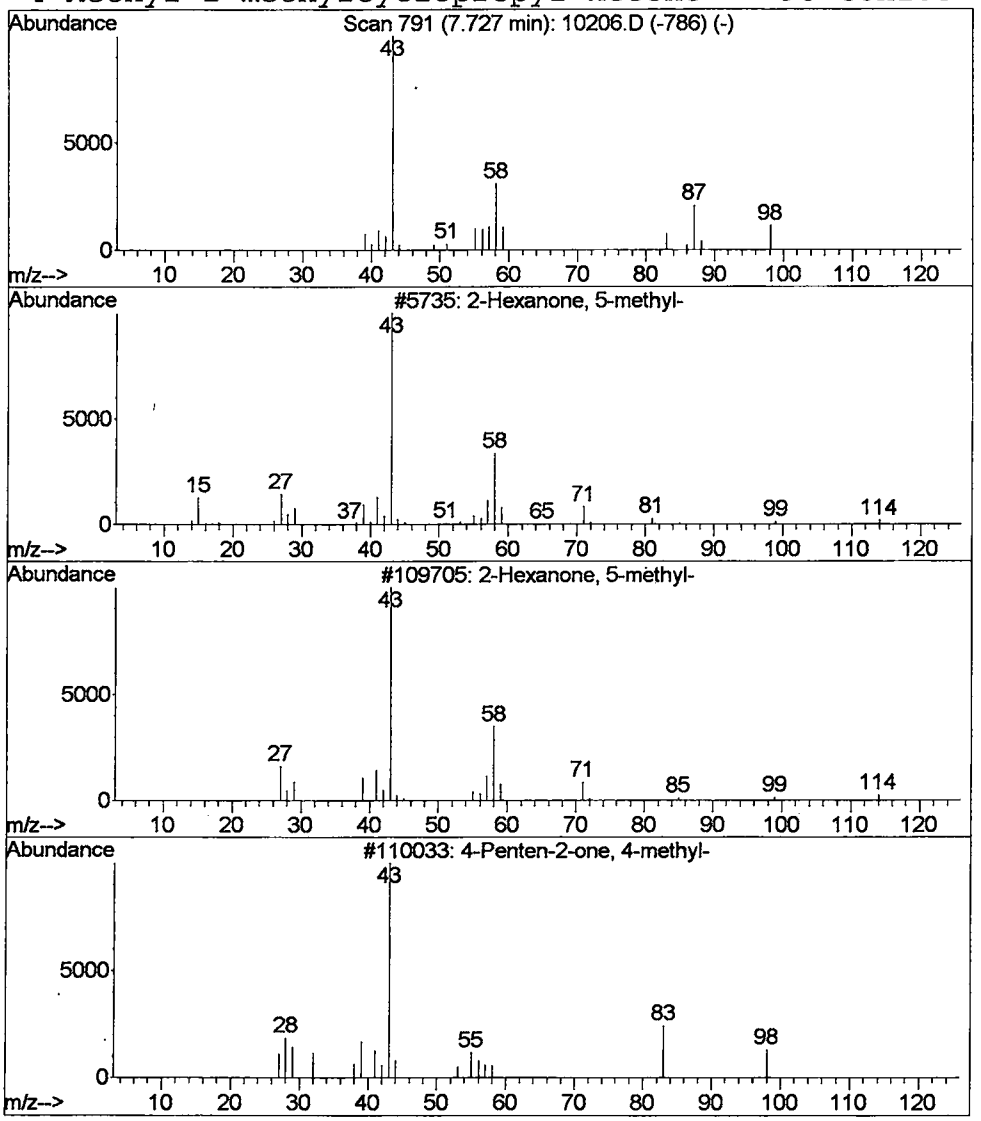
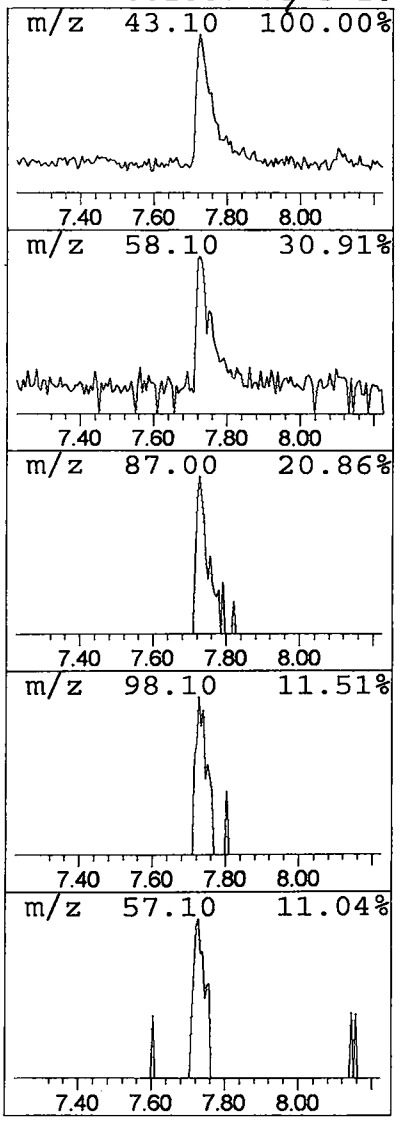
Peak Number 4 2-Hexanone, 5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	0.25 ug/L	211281	1,4-Dichlorobenzene-d4	9.94

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	25
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	25
3	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	17
4	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	10





Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
Sample : 5/10 eh Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.e

Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

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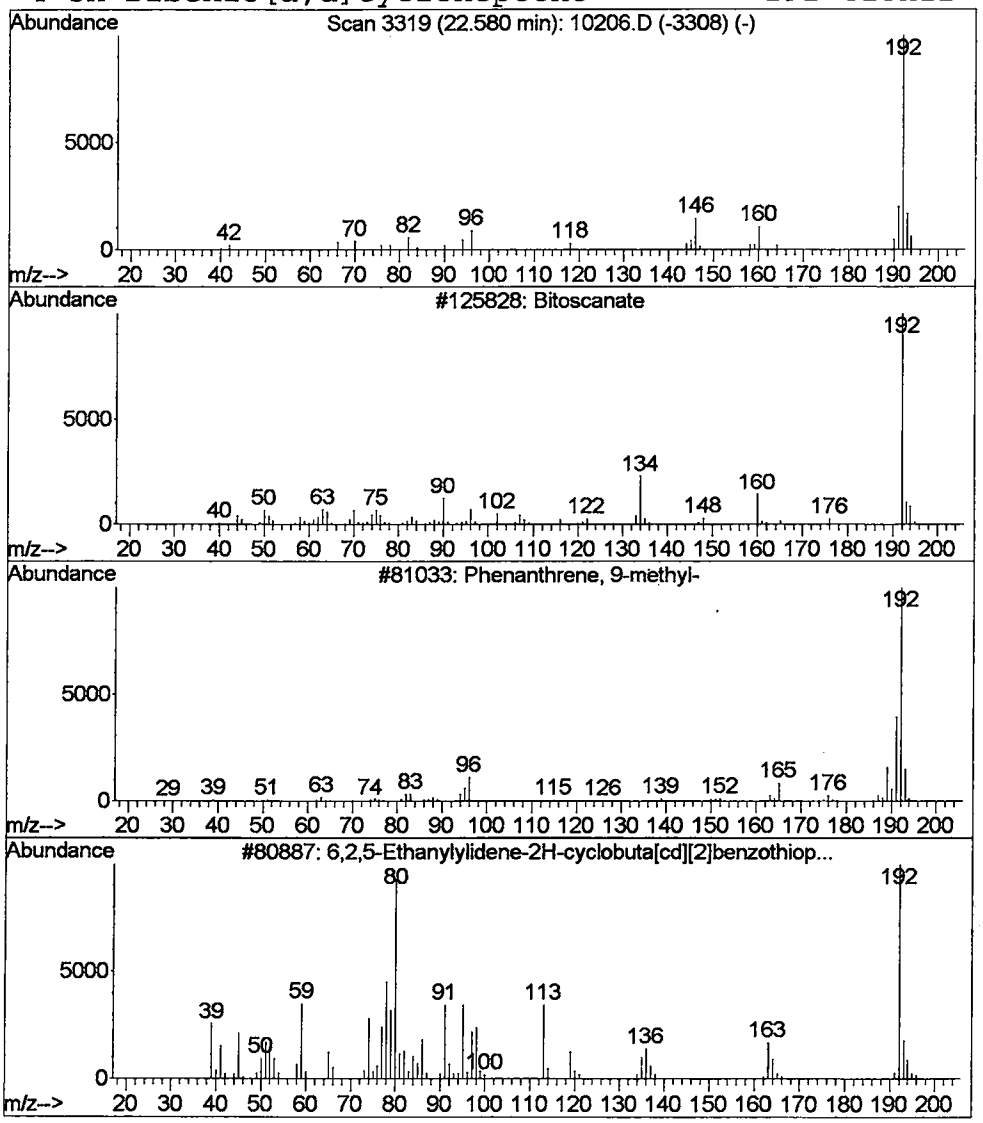
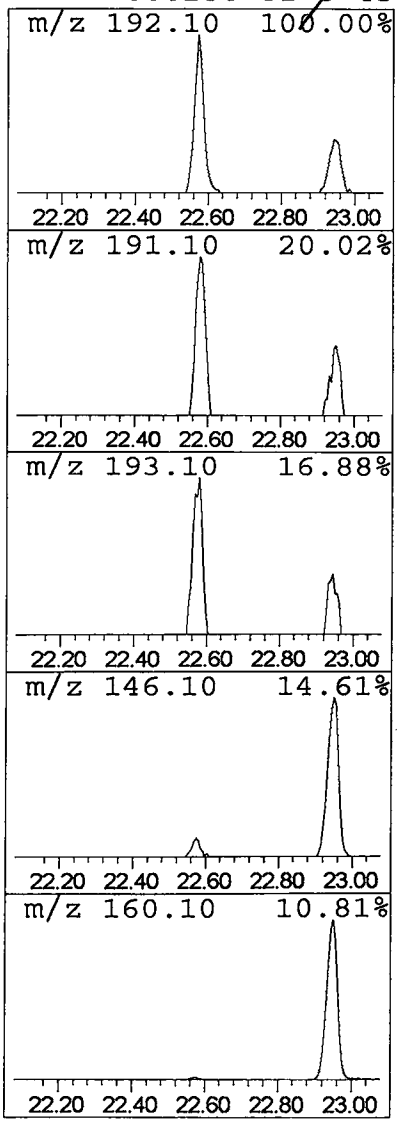
Peak Number 5 Bitoscanate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	0.30 ug/L	357129	Phenanthranene-d10	22.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bitoscanate	192	C8H4N2S2	004044-65-9	53
2	Phenanthrene, 9-methyl-	192	C15H12	000883-20-5	53
3	6,2,5-Ethanylylidene-2H-cyclobut...	192	C11H12OS	019086-86-3	47
4	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	45





Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
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Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

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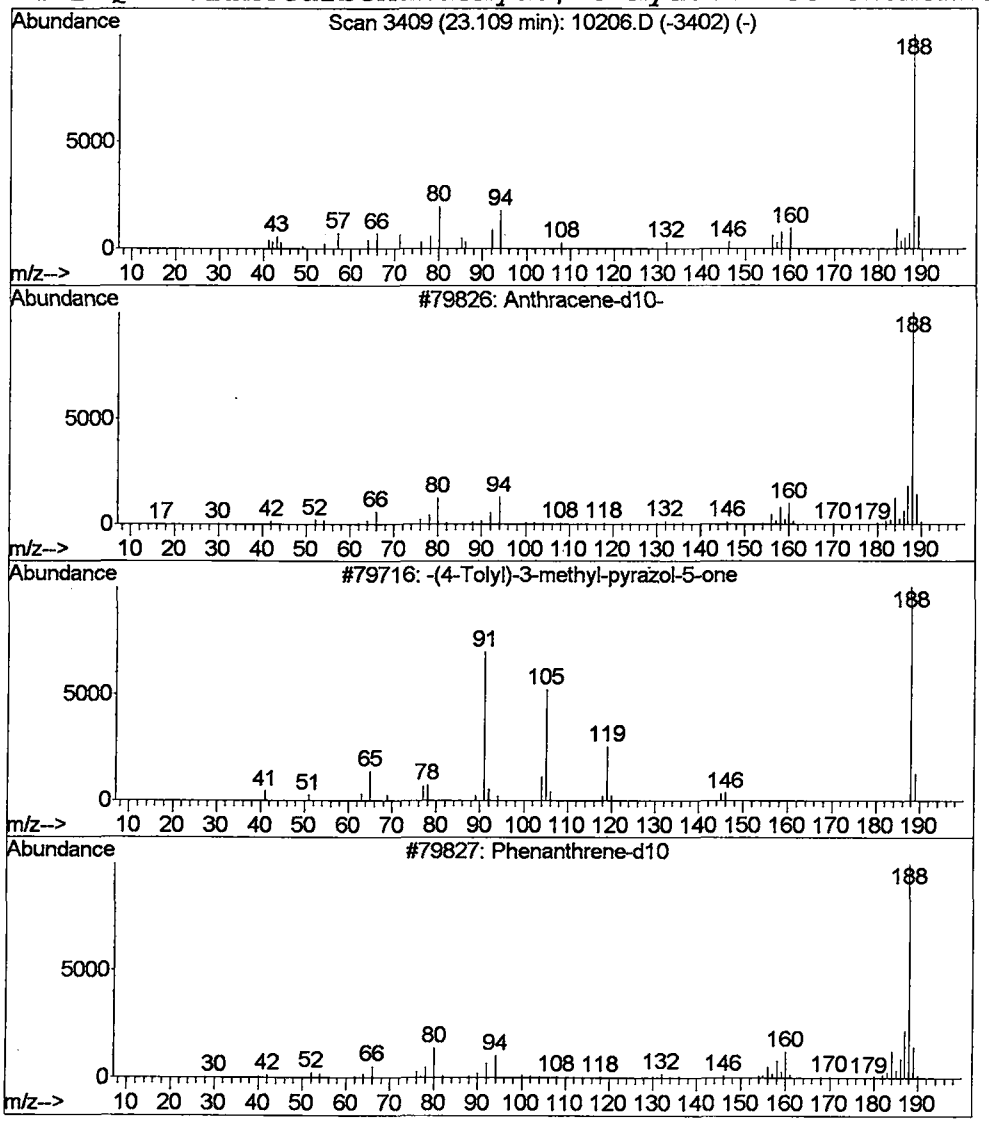
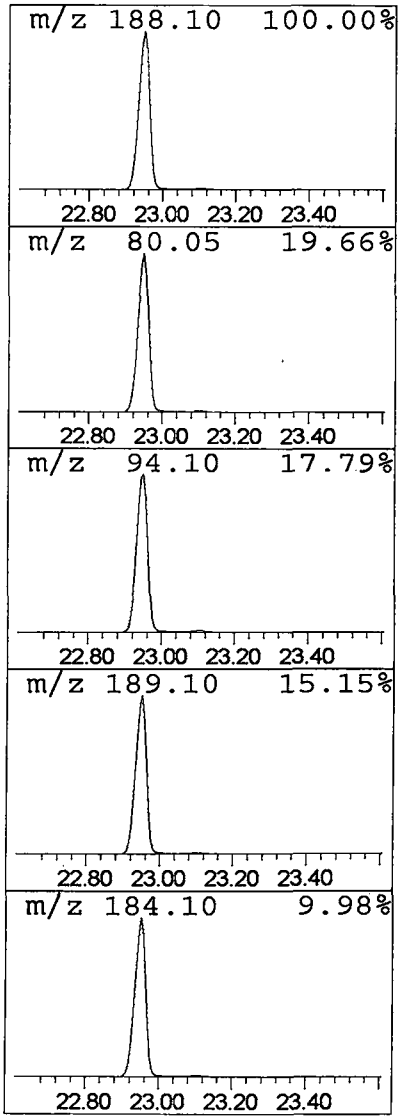
Peak Number 6 Anthracene-d10- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.11	0.36 ug/L	437602	Phenanthranene-d10	22.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthracene-d10-	188	C14D10	001719-06-8	91
2	-(4-Tolyl)-3-methyl-pyrazol-5-one	188	C11H12N2O	035496-19-6	47
3	Phenanthrene-d10	188	C14D10	001517-22-2	38
4	2-Quinolinecarboxaldehyde, 8-hyd...	188	C10H8N2O2	005603-22-5	37





Data File : C:\MSDCHEM\1\DATA\051602\10206.D Vial: 7
Acq On : 16 May 2002 7:25 pm Operator: Mclean
Sample : 5/10 eh Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.e

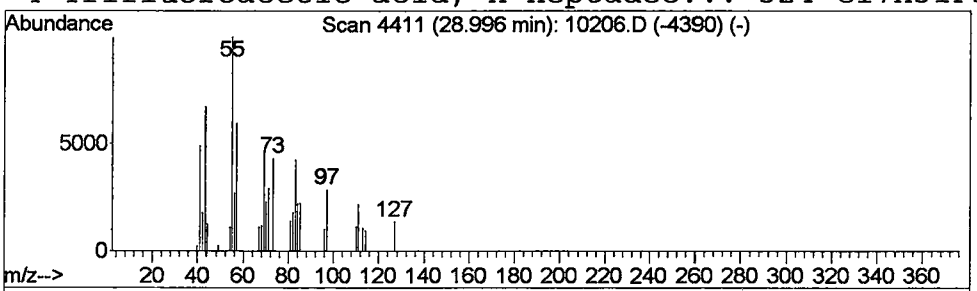
Quant Method : C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title : 508 Modified GC/MS scan
Library : C:\DATABASE\NIST98.L

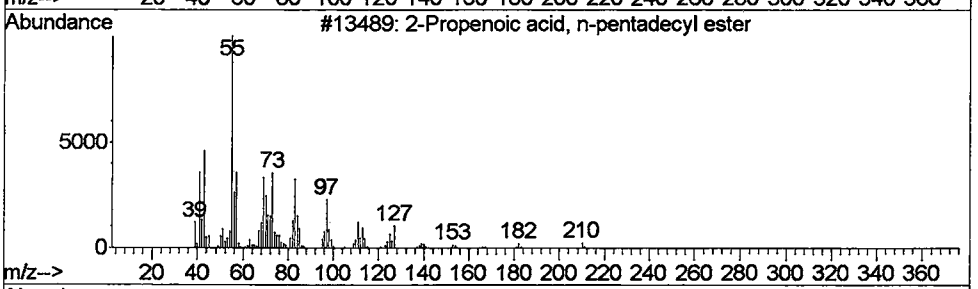
****

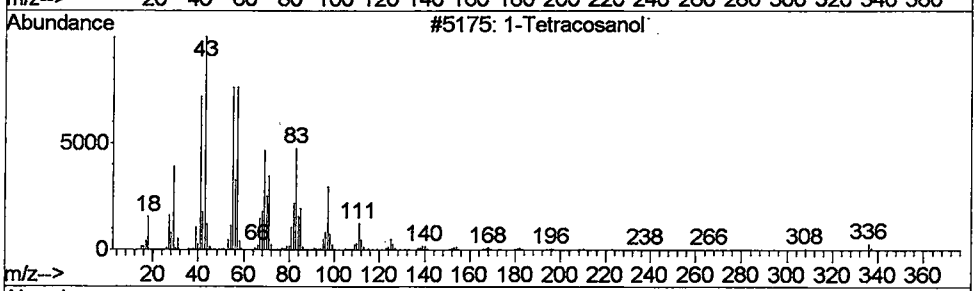
Peak Number 7 2-Propenoic acid, n-pentade... Concentration Rank 7

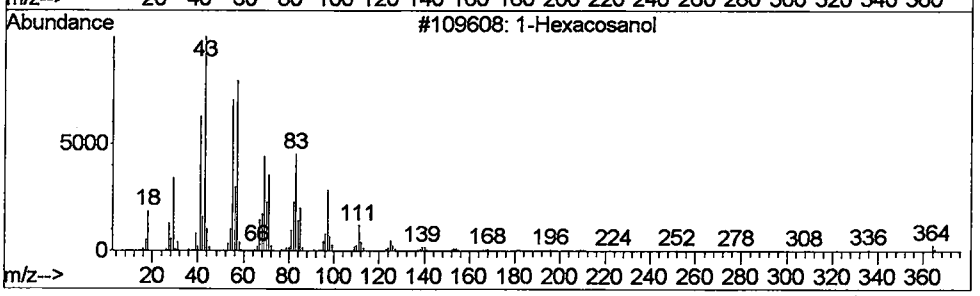
R.T.	EstConc	Area	Relative to ISTD	R.T.
29.00	0.22 ug/L	220311	Chrysene-d12	30.81

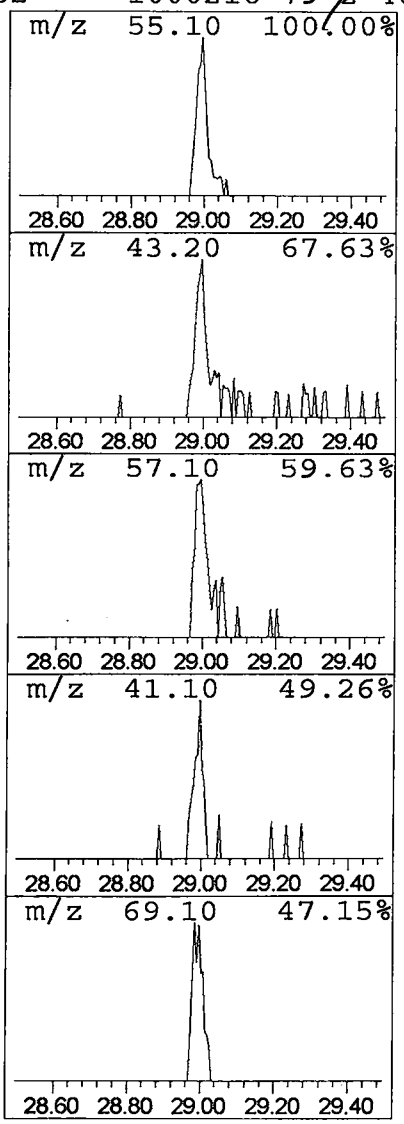
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propenoic acid, n-pentadecyl e...	282	C18H34O2	1000245-64-0	53
2	1-Tetracosanol	354	C24H50O	000506-51-4	46
3	1-Hexacosanol	382	C26H54O	000506-52-5	46
4	Trifluoroacetic acid, n-heptadec...	324	C17H31F3O2	1000216-79-2	46











Tentatively Identified Compound (TIC) Summary

Operator ID: Mclean Date Acquired: 16 May 2002 7:25 pm
Data File: C:\MSDCHEM\1\DATA\051602\10206.D
Name: 5/10 eh
Misc:
Method: C:\MSDCHEM\1\METHODS\050102.M (Chemstation Integrator)
Title: 508 Modified GC/MS scan
Library Searched: C:\DATABASE\NIST98.L

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
Acetonitrile, dic...	3.60	0.3	ug/L	221266	1	9.94	33579400	40.0
2-Chloroethanol	3.72	0.3	ug/L	276938	1	9.94	33579400	40.0
2-Pentanone, 4-hy...	5.97	17.1	ug/L	14350400	1	9.94	33579400	40.0
2-Hexanone, 5-met...	7.73	0.3	ug/L	211281	1	9.94	33579400	40.0
Bitoscanate	22.58	0.3	ug/L	357129	4	22.95	48031100	40.0
Anthracene-d10-	23.11	0.4	ug/L	437602	4	22.95	48031100	40.0
2-Propenoic acid,...	29.00	0.2	ug/L	220311	5	30.81	39520800	40.0