User: Vinci, David L
Westchester Dept. of Labs & Research
Date: 04/19/2002 Time: 10:38:06

Sample: AE06795
Analysis: $GCMS GCMS Scan For Unknowns
Units: ug
Started: 4/19/02 10:35 Ended: 4/19/02 10:35 Analyst: DLV
Page: 1

	Component Name	Viol	Result	Qualifier	MDL
1	Other unknown compounds		.		
2	Surr_2,4-DDD		104		5.0

Scott
3/19/2
MeOH

Comments for Sample AE06795 - Analysis $GCMS

Westchester Dept. of Labs & Research
User: Vinci, David L
Date: 04-19-2002 Time: 10:40:12

The GCMS scan, from 35 to 550 amu, reveals the presence of several low level unidentified compounds in the retention time range of 32 minutes to 33.5 minutes.

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\041602\6795.D Vial: 13
Acq On : 16 Apr 2002 6:31 pm Operator: Bohlk
Sample : SAMPLE 6795 3/21/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: BENZO.P
Quant Time: Apr 18 16:29:06 2002 Quant Results File: 5080402BBC.RES

Quant Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Last Update : Tue Apr 16 18:27:45 2002
Response via : Initial Calibration
DataAcq Meth : 508SCAN

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	9.41	152	483805	40.00	ug/L	0.00
10) Naphthalene-d8	12.88	136	2146980	40.00	ug/L	0.00
17) Acenaphthene-d10	17.99	164	1198552	40.00	ug/L	0.00
30) Phenanthrene-d10	22.34	188	1727058	40.00	ug/L	0.00
39) Chrysene-d12	30.14	240	1435566	40.00	ug/L	-0.01
45) Perylene-d12	34.01	264	875009	40.00	ug/L	0.00
System Monitoring Compounds						
28) TCMX (SURR)	0.00	244	0	0.00	ug/L	
Spiked Amount 10.000			Recovery = 0.00%			
38) 2,4-DDD (SURR)	27.27	235	134087	10.43	ug/L	0.00
Spiked Amount 10.000			Recovery = 104.30%			
Target Compounds						Qvalue
2) N-nitroso-dimethyl amine	0.00	74	0	N.D. d		
3) bis(2-chloroethyl) ether	0.00	93	0	N.D.		
4) 1,3 - Dichlorobenze	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-Chloropr	0.00	45	0	N.D.		
8) N-Nitroso-di-n-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) Naphthalene	0.00	128	0	N.D.		
16) Hexachlorobutadiene	0.00	225	0	N.D.		
18) Hexachlorocyclopentadiene	0.00	237	0	N.D.		
19) 2-chloronaphthalene	0.00	162	0	N.D.		
20) Dimethylphthalate	0.00	163	0	N.D.		
21) 2,6-Dinitrotoluene	0.00	165	0	N.D. d		
22) Acenaphthylene	0.00	152	0	N.D.		
23) Acenaphthene	0.00	153	0	N.D.		
24) 2,4-Dinitrotoluene	0.00	165	0	N.D.		
25) Diethylphthalate	0.00	149	0	N.D.		
26) 4-Chlorophenyl-phenyl ethe	0.00	204	0	N.D.		
27) Fluorene	0.00	166	0	N.D.		
29) Azobenzen/ 1,2-Diphenylhyd	0.00	77	0	N.D.		
31) N-Nitrosodiphenylamine	0.00	169	0	N.D.		
32) 4-Bromophenyl-phenyl ether	0.00	248	0	N.D.		
33) Hexachlorobenzene	0.00	284	0	N.D.		
34) Phenanthrene	0.00	178	0	N.D.		
35) Anthracene	0.00	178	0	N.D.		
36) Di-n-butylphthalate	0.00	149	0	N.D. d		
37) Fluoranthene	0.00	202	0	N.D.		
40) Pyrene	0.00	202	0	N.D.		
41) Butylbenzylphthalate	0.00	149	0	N.D.		
42) Benzo (a) antracene	0.00	228	0	N.D. d		
43) Bis (2-ethylhexyl) phthala	30.77	149	141226	3.98	ug/L	96
44) Chrysene	0.00	228	0	N.D. d		

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

Quantitation Report (QT Reviewed)

Data File : C:\MSDCHEM\1\DATA\041602\6795.D Vial: 13
Acq On : 16 Apr 2002 6:31 pm Operator: Bohlk
Sample : SAMPLE 6795 3/21/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: BENZO.P
Quant Time: Apr 18 16:29:06 2002 Quant Results File: 5080402BBC.RES

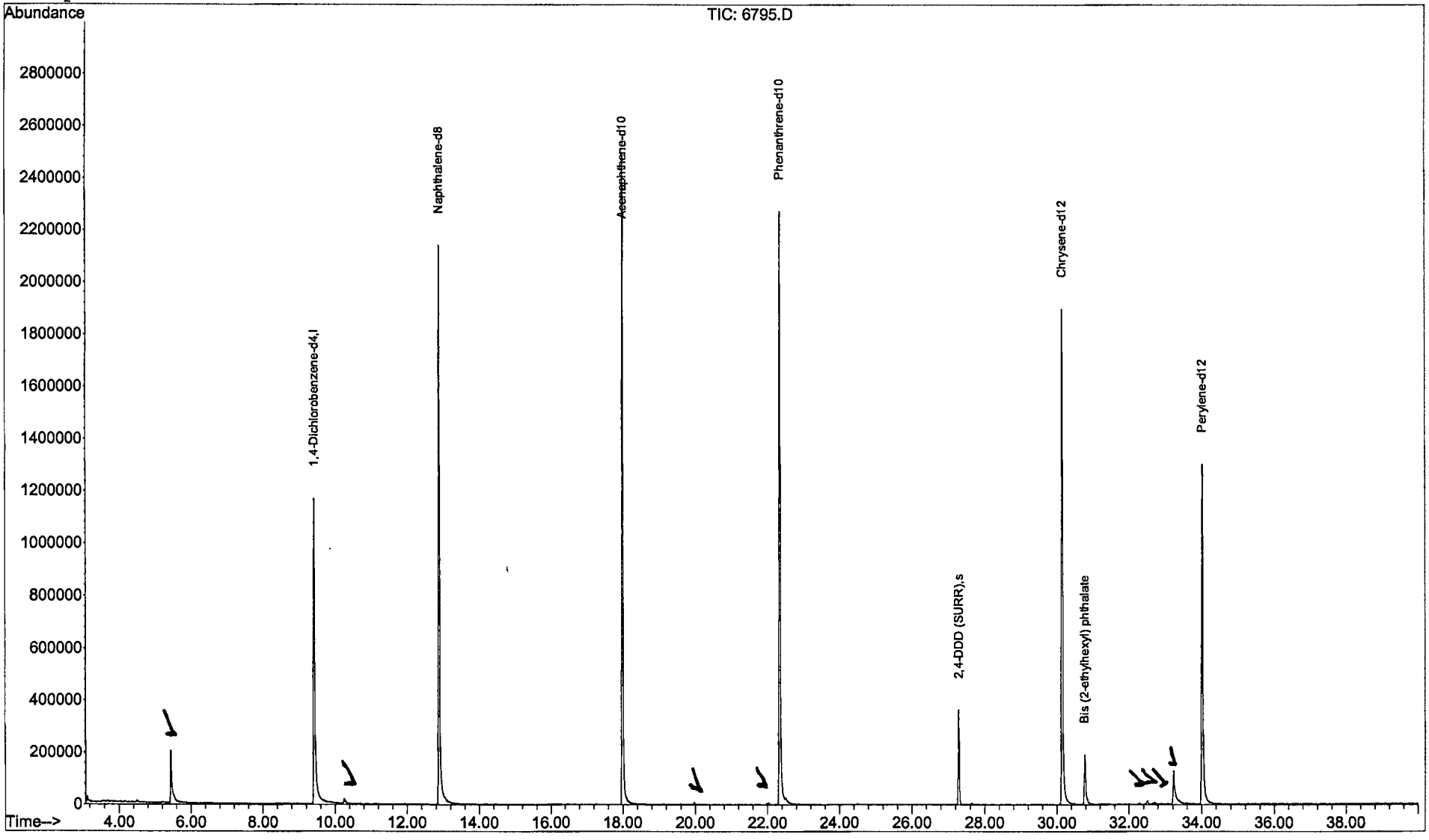
Quant Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Last Update : Tue Apr 16 18:27:45 2002
Response via : Initial Calibration
DataAcq Meth : 508SCAN

Compound	R.T.	QIon	Response	Conc Unit	Qvalue
46) Di-n-Octylphthalate	0.00	149	0	N.D.	
47) Benzo (b) fluoranthene	0.00	252	0	N.D.	
48) Benzo (k) fluoranthene	0.00	252	0	N.D.	
49) Benzo (a) pyrene	0.00	252	0	N.D.	d
50) Indeno (1,2,3-cd) pyrene	0.00	276	0	N.D.	
51) Dibenz (a,h) anthracene	0.00	278	0	N.D.	
52) Benzo (g,h,i) perylene	0.00	276	0	N.D.	

(#) = qualifier out of range (m) = manual integration
6795.D 5080402BBC.M Thu Apr 18 16:30:27 2002 Page 2

Data File : C:\MSDCHEM\1\DATA\041602\6795.D Vial: 13
Acq On : 16 Apr 2002 6:31 pm Operator: Bohlk
Sample : SAMPLE 6795 3/21/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: BENZO.P
Quant Time: Apr 18 16:30 2002 Quant Results File: 5080402BBC.RES

Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Last Update : Tue Apr 16 18:27:45 2002
Response via : Initial Calibration



Data File : C:\MSDCHEM\1\DATA\041602\6795.D Vial: 13
Acq On : 16 Apr 2002 6:31 pm Operator: Bohlk
Sample : SAMPLE 6795 3/21/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.P

Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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

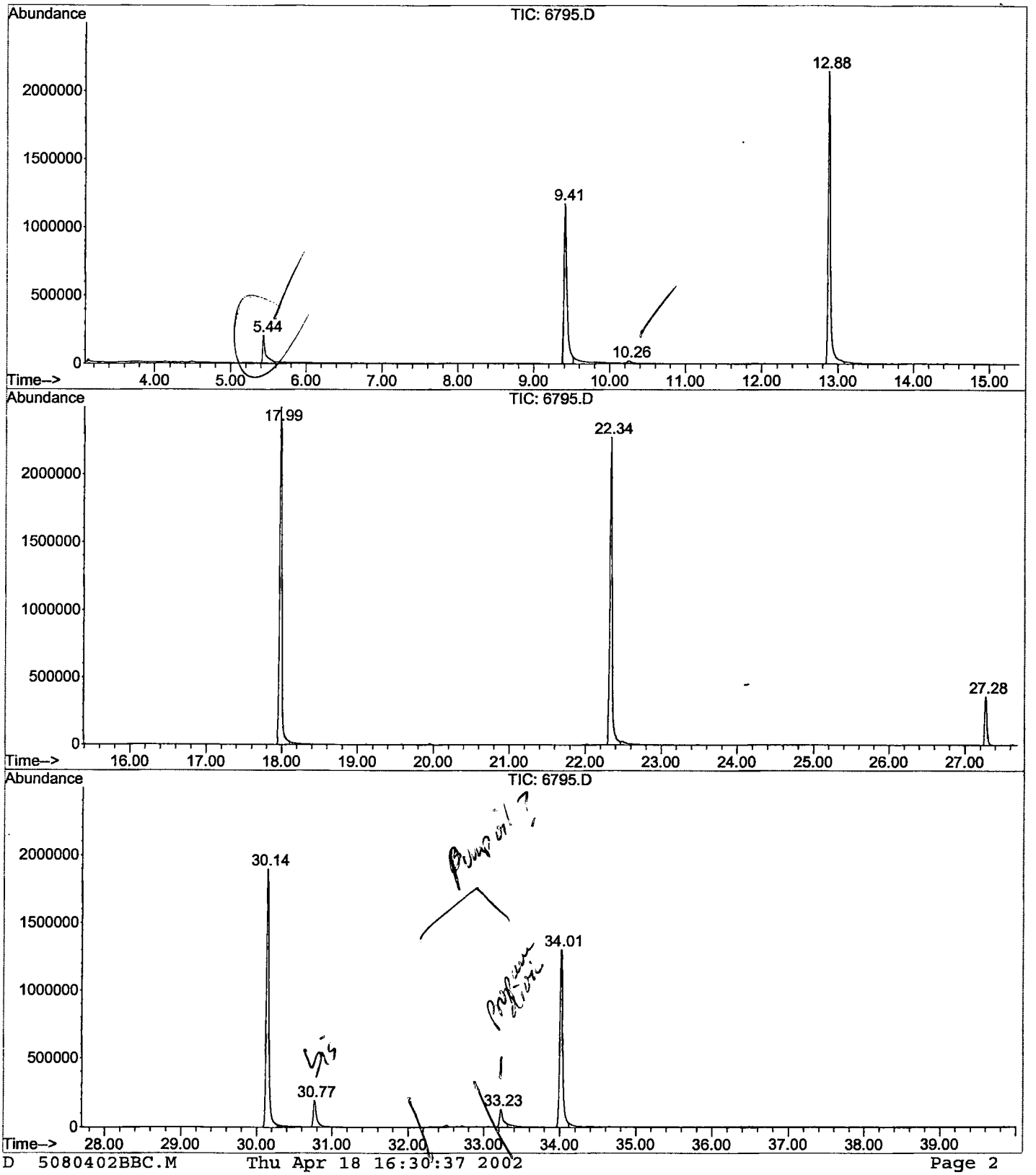
Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.435	396	401	428	rBV	200571	575173	11.25%	2.060%
2	9.407	1071	1077	1096	rBV	1168279	3055947	59.76%	10.944%
3	10.259	1215	1222	1237	rBV5	16865	54876	1.07%	0.197%
4	12.880	1661	1668	1702	rBV	2140121	4698008	91.88%	16.825%
5	17.986	2528	2537	2557	rBV	2493499	5113339	100.00%	18.312%
6	22.339	3269	3278	3299	rBV2	2272862	4958548	96.97%	17.758%
7	27.281	4112	4119	4136	rVB	361776	727020	14.22%	2.604%
8	30.142	4591	4606	4630	rBV2	1896925	4510248	88.21%	16.153%
9	30.765	4704	4712	4731	rBV2	189964	543078	10.62%	1.945%
10	33.227	5123	5131	5145	rBV4	126995	419024	8.19%	1.501%
11	34.014	5255	5265	5282	rBV	1301733	3267619	63.90%	11.702%

Sum of corrected areas: 27922880

LSC Report - Integrated Chromatogram

File : C:\MSDCHEM\1\DATA\041602\6795.D
Operator : Bohlk
Acquired : 16 Apr 2002 6:31 pm using AcqMethod 508SCAN
Instrument : Instrumen
Sample Name: SAMPLE 6795 3/21/02
Misc Info :
Vial Number: 13
Quant File :5080402BBC.RES (RTE Integrator)



Data File : C:\MSDCHEM\1\DATA\041602\6795.D Vial: 13
Acq On : 16 Apr 2002 6:31 pm Operator: Bohlk
Sample : SAMPLE 6795 3/21/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.P

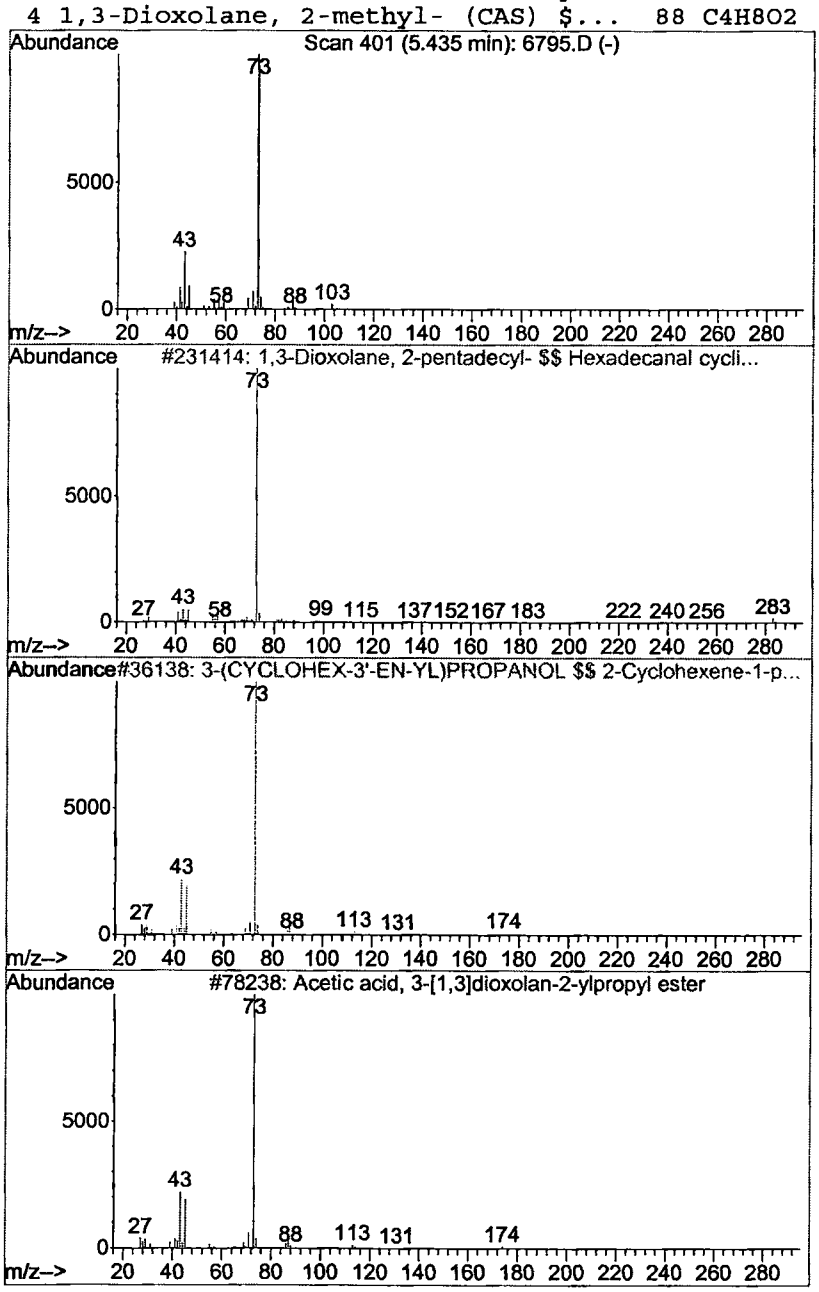
Quant Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Library : C:\DATABASE\WILEY7N.L

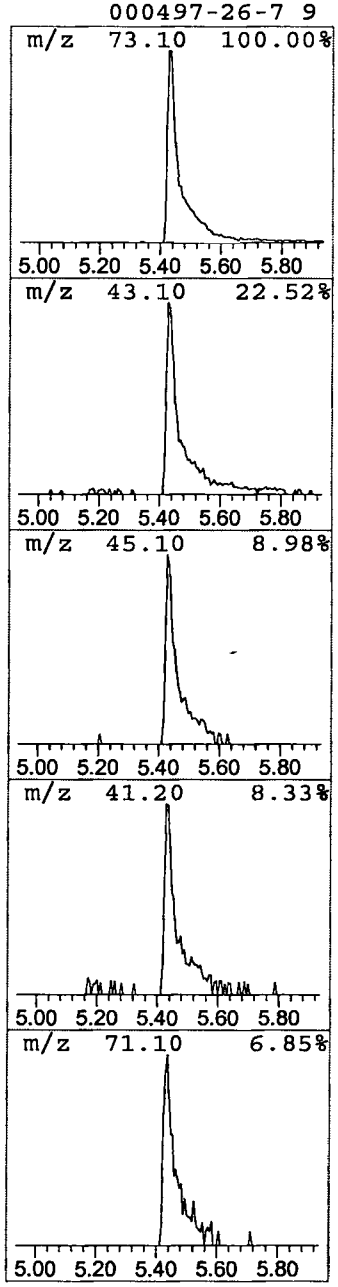
****

Peak Number 1 1,3-Dioxolane, 2-pentadecyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.44	7.53 ug/L	575173	1,4-Dichlorobenzene-d4	9.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-pentadecyl- $$ ...	284	C18H36O2	004360-57-0	38
2	3-(CYCLOHEX-3'-EN-YL)PROPANOL $$...	174	C8H14O4	015745-87-6	36
3	Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	000000-00-0	36
4	1,3-Dioxolane, 2-methyl- (CAS) $...	88	C4H8O2	000497-26-7	9





Data File : C:\MSDCHEM\1\DATA\041602\6795.D Vial: 13
Acq On : 16 Apr 2002 6:31 pm Operator: Bohlk
Sample : SAMPLE 6795 3/21/02 Inst : Instrumen
Misc : Multiplr: 1.00
MS Integration Params: LSCINT.P

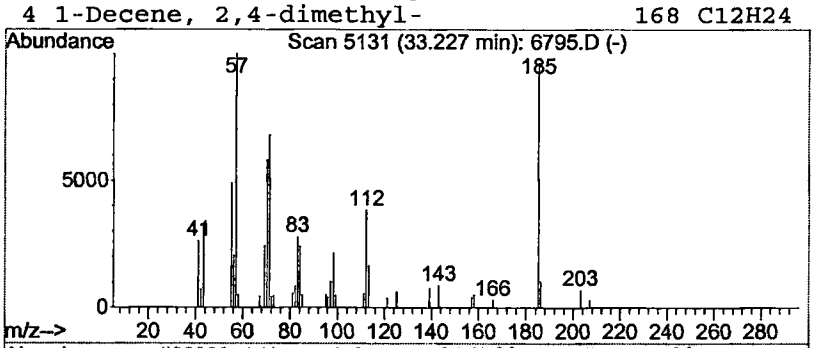
Quant Method : C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title : Quantitation For Method 508gcscan
Library : C:\DATABASE\WILEY7N.L

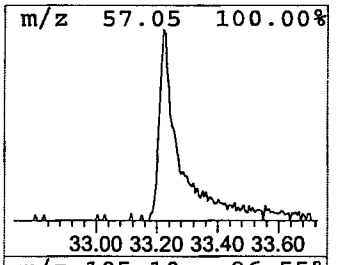
****

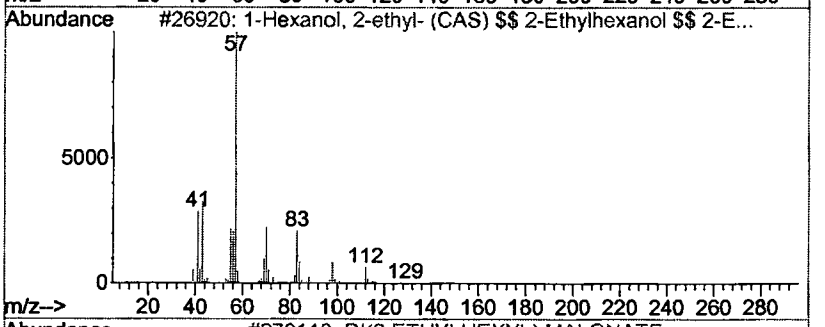
Peak Number 2 1-Hexanol, 2-ethyl- (CAS) $... Concentration Rank 2

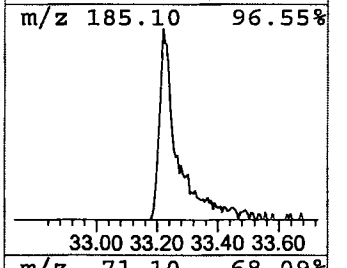
R.T.	EstConc	Area	Relative to ISTD	R.T.
33.23	5.13 ug/L	419024	Perylene-d12	34.01

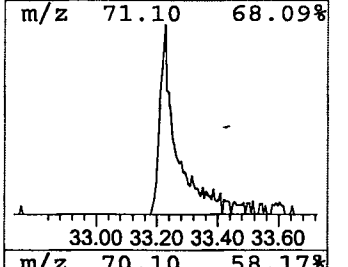
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl- (CAS) $$ 2-E...	130	C8H18O	000104-76-7	38
2	DI(2-ETHYLHEXYL) MALONATE	328	C19H36O4	000000-00-0	38
3	Propanedioic acid, hexyl-, dieth...	244	C13H24O4	005398-10-7	38
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	35

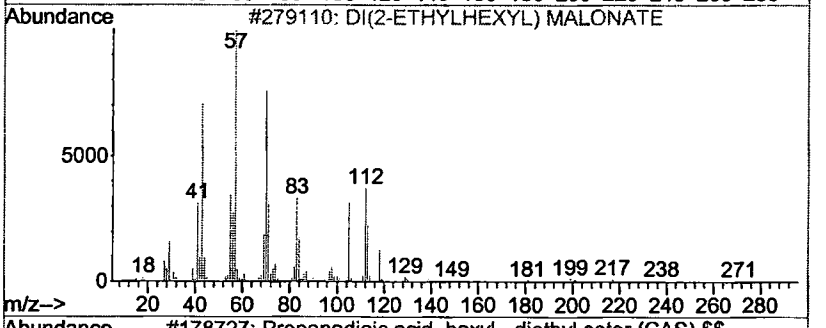


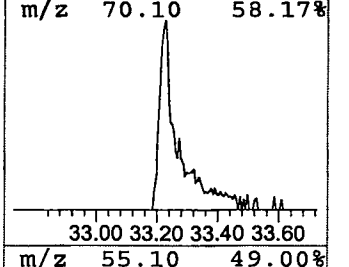


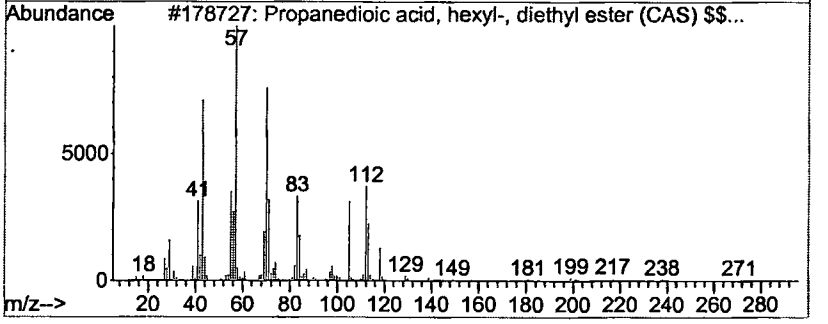


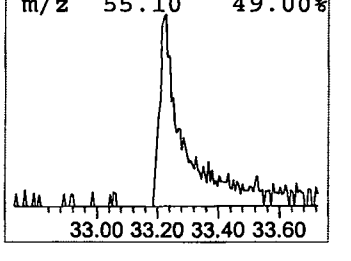








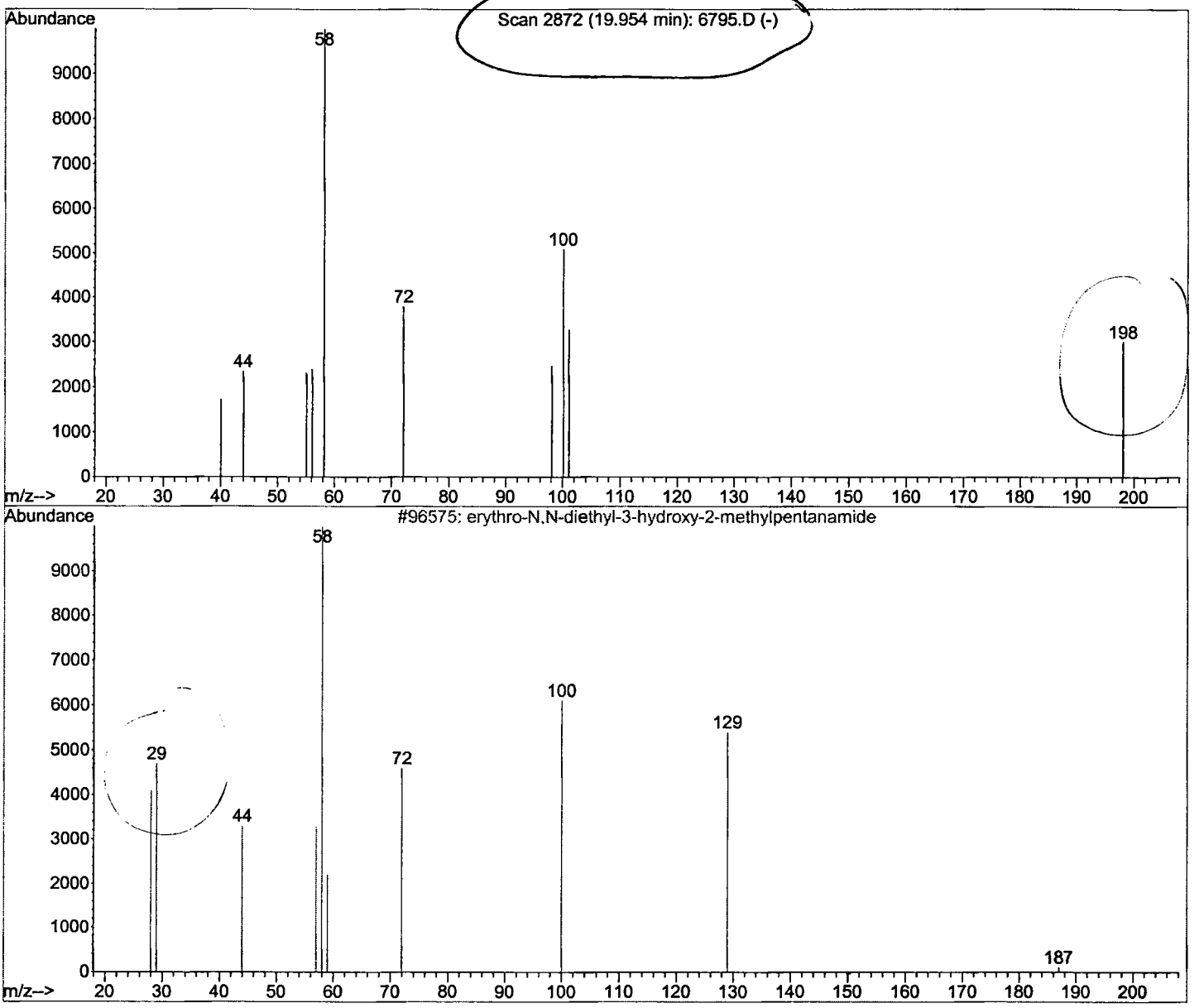




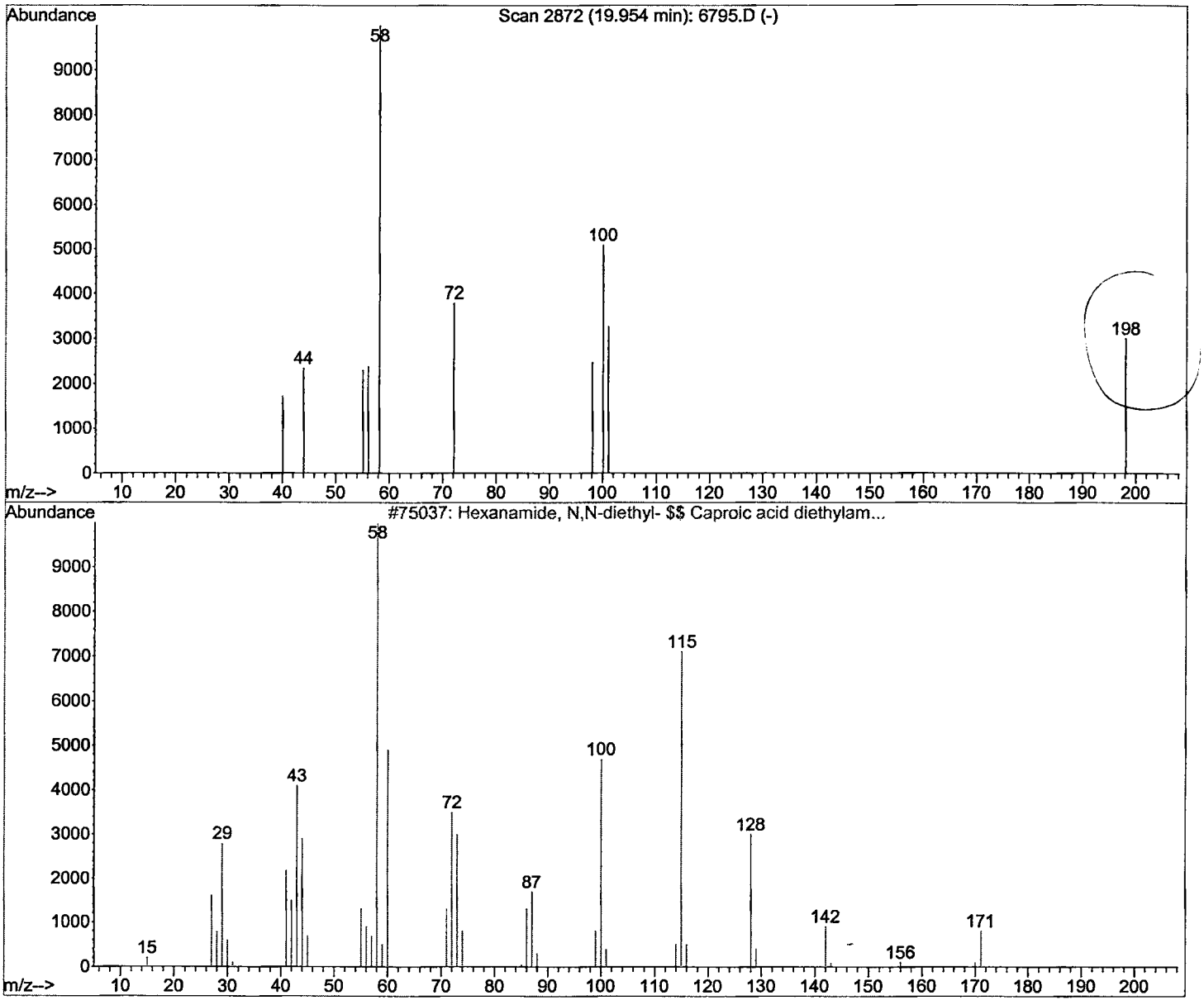
Operator ID: Bohlk Date Acquired: 16 Apr 2002 6:31 pm
Data File: C:\MSDCHEM\1\DATA\041602\6795.D
Name: SAMPLE 6795 3/21/02
Misc:
Method: C:\MSDCHEM\1\5973N\5080402BBC.M (RTE Integrator)
Title: Quantitation For Method 508gcscan
Library Searched: C:\DATABASE\WILEY7N.L

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
1,3-Dioxolane, 2-...	5.44	7.5	ug/L	575173	1	9.41	3055950	40.0
1-Hexanol, 2-ethy...	33.23	5.1	ug/L	419024	6	34.01	3267620	40.0

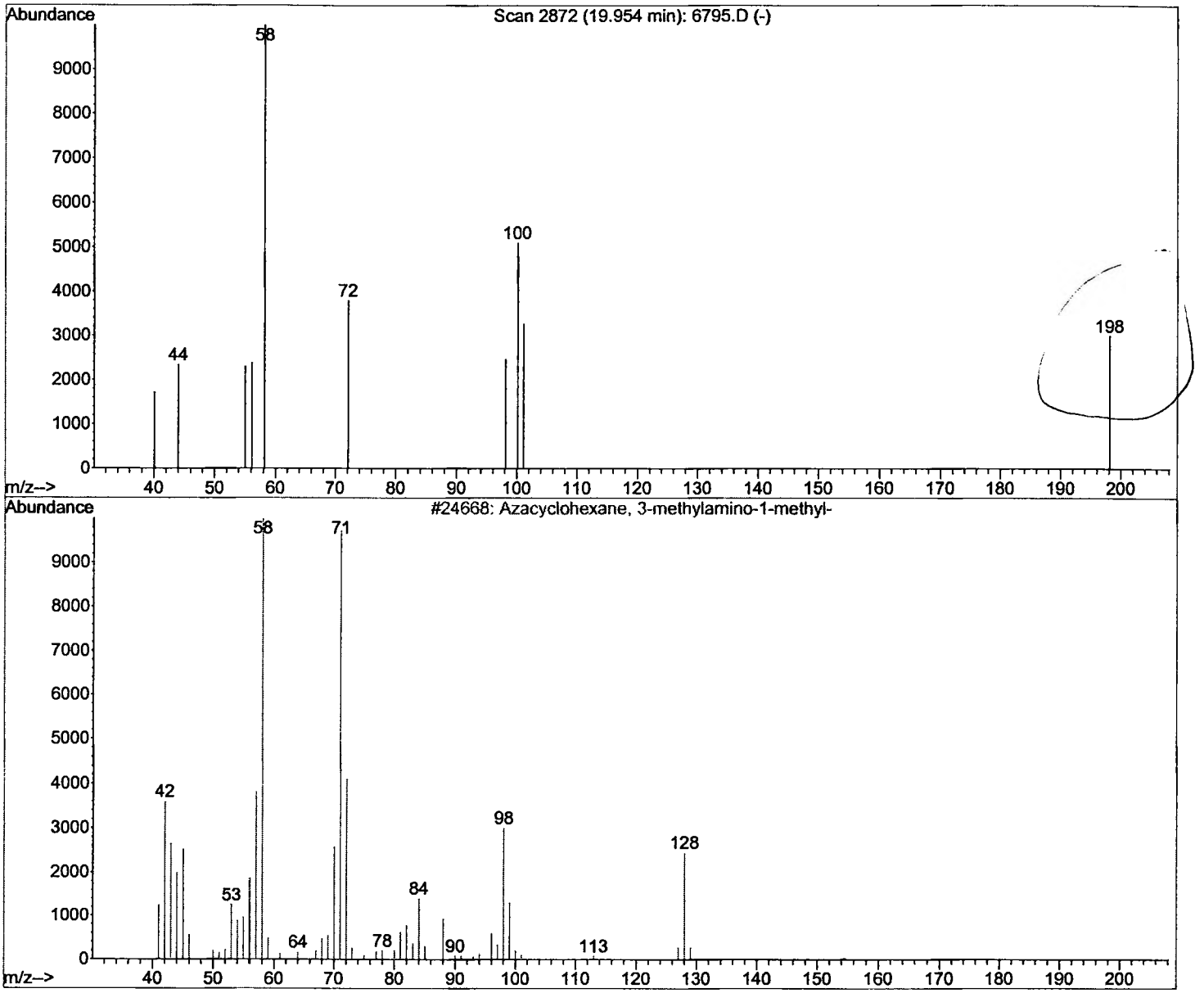
Library Searched : C:\Database\wiley7n.l
Quality : 36
ID : erythro-N,N-diethyl-3-hydroxy-2-methylpentanamide



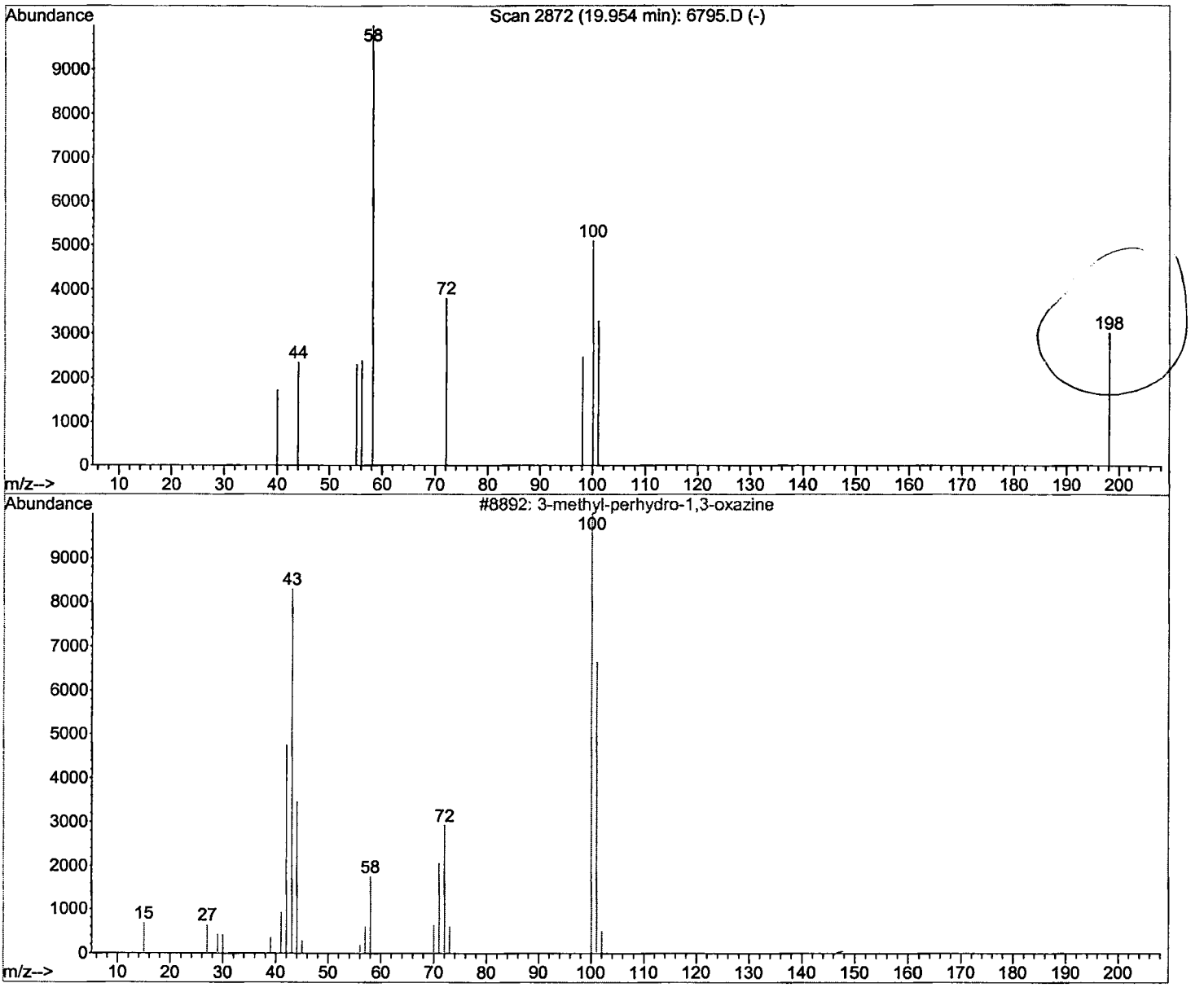
Library Searched : C:\Database\wiley7n.l
Quality : 36
ID : Hexanamide, N,N-diethyl- $$ Caproic acid diethylamide $$ N,N-Diethylhexanamide $$ R 31



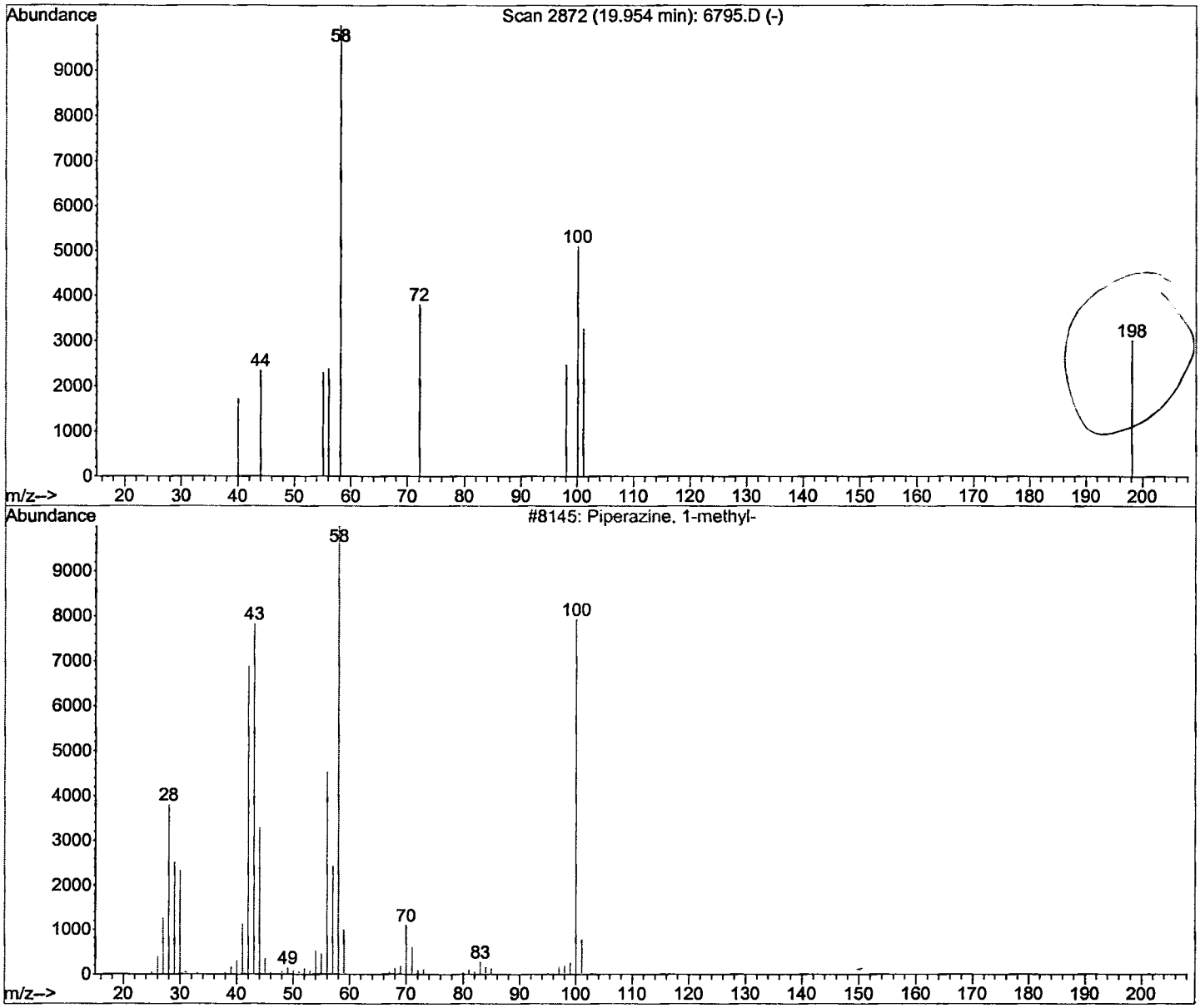
Library Searched : C:\Database\wiley7n.l
Quality : 28
ID : Azacyclohexane, 3-methylamino-1-methyl-



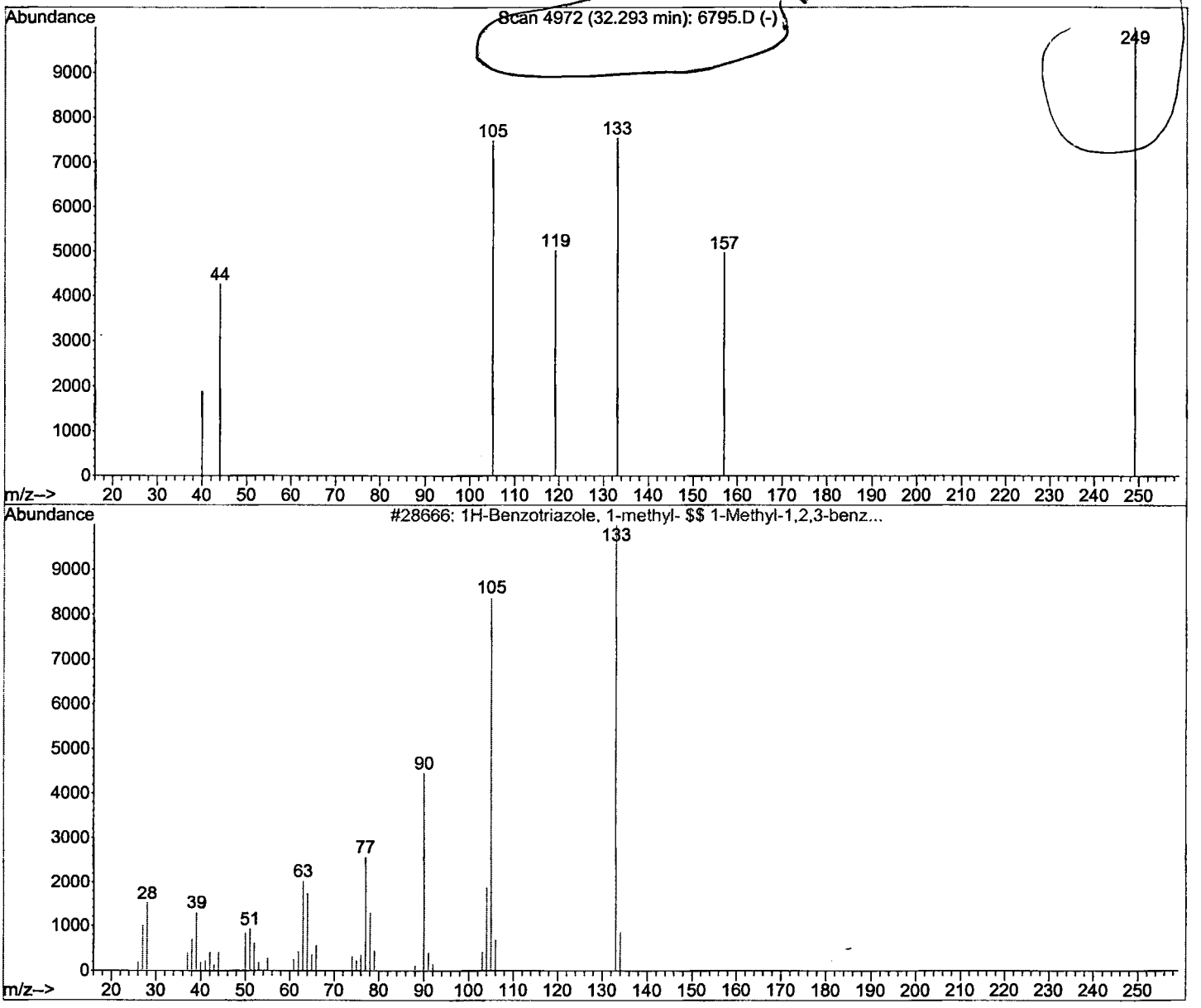
Library Searched : C:\Database\wiley7n.l
Quality : 9
ID : 3-methyl-perhydro-1,3-oxazine



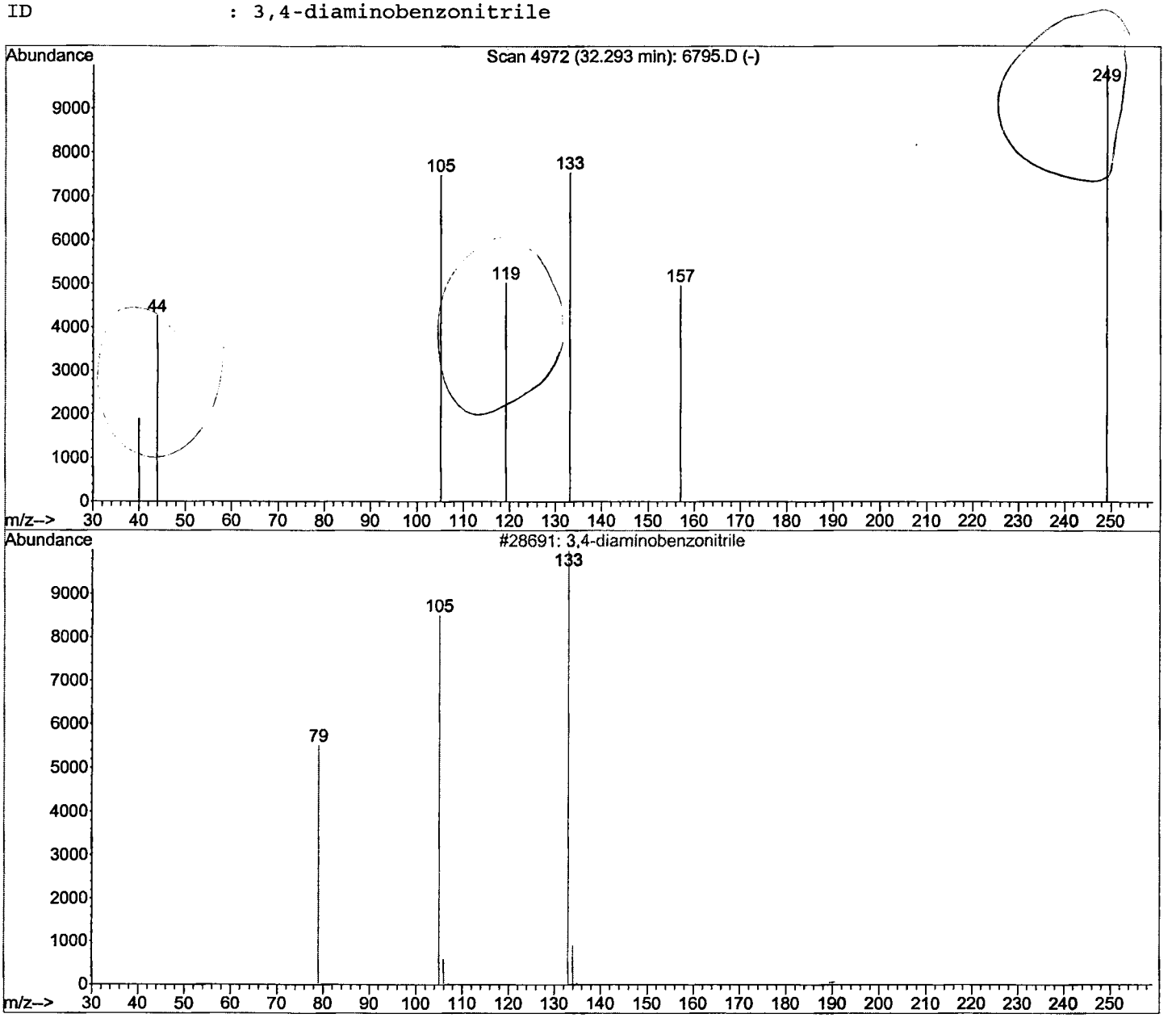
Library Searched : C:\Database\wiley7n.l
Quality : 9
ID : Piperazine, 1-methyl-



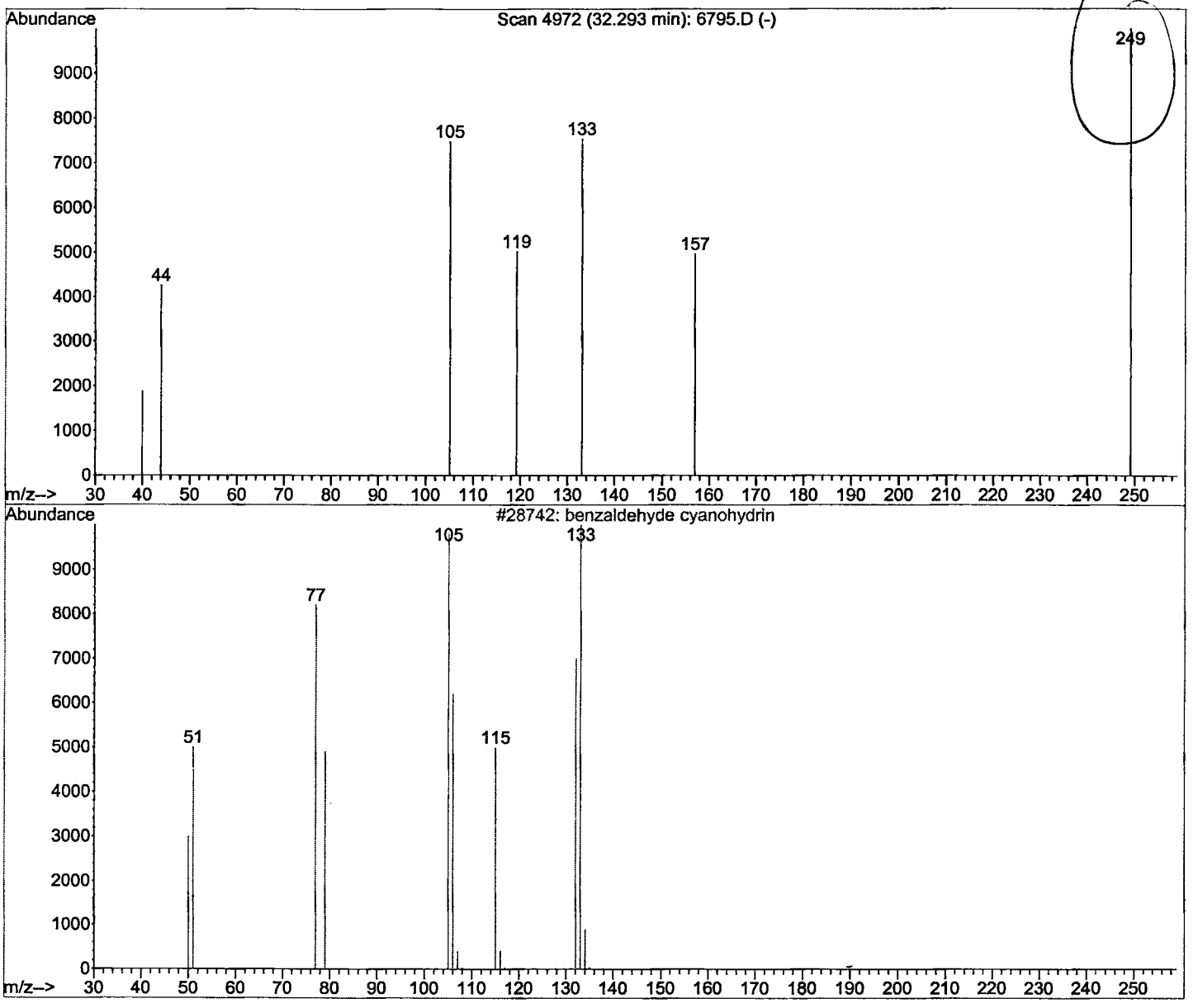
Library Searched : C:\Database\wiley7n.l
Quality : 4
ID : 1H-Benzotriazole, 1-methyl- $$ 1-Methyl-1,2,3-benzotriazole $$ 1-Methylbenzotriazole $$ 1-Methyl-1H-benzotriazole



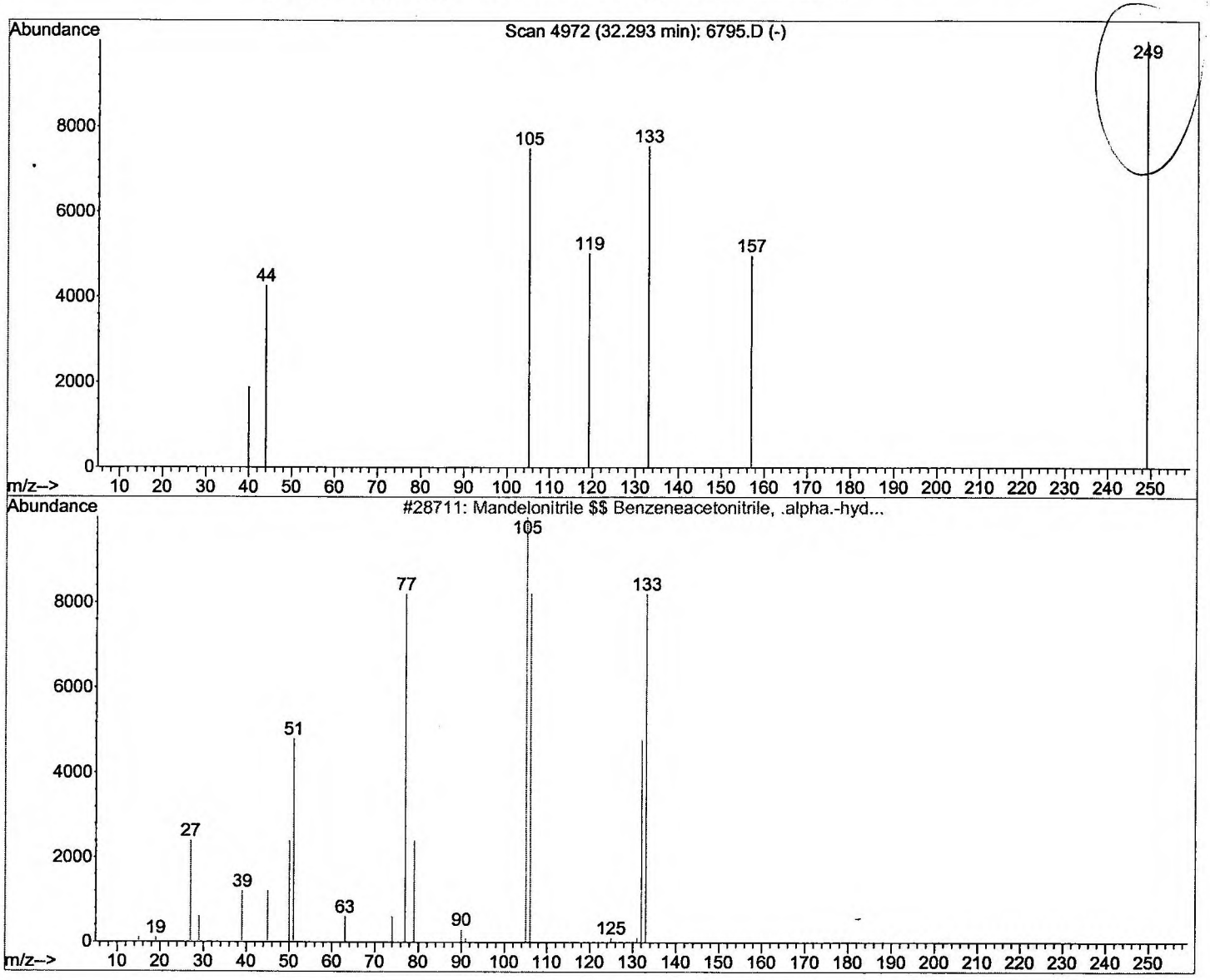
Library Searched : C:\Database\wiley7n.l
Quality : 4
ID : 3,4-diaminobenzonitrile



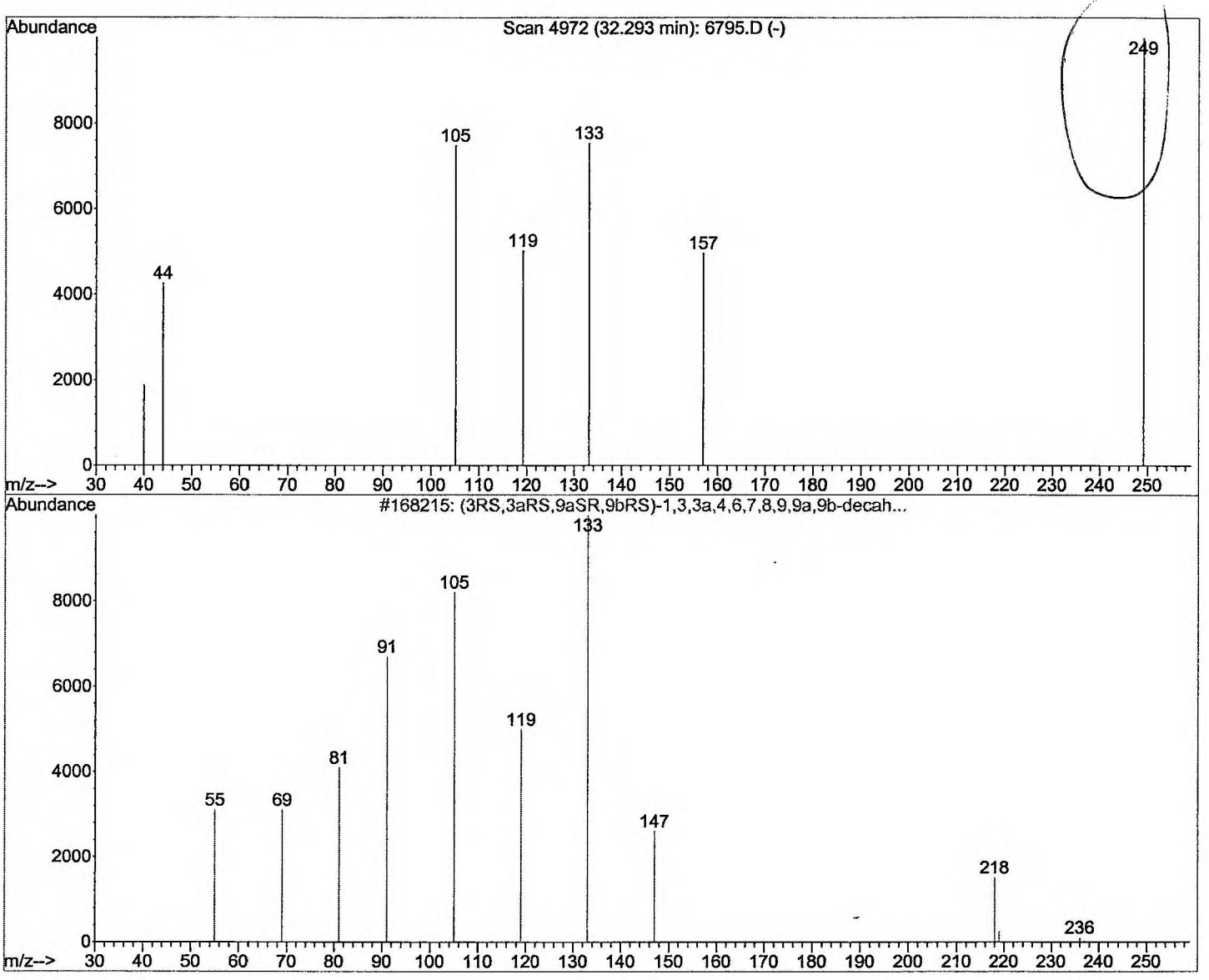
Library Searched : C:\Database\wiley7n.l
Quality : 4
ID : benzaldehyde cyanohydrin



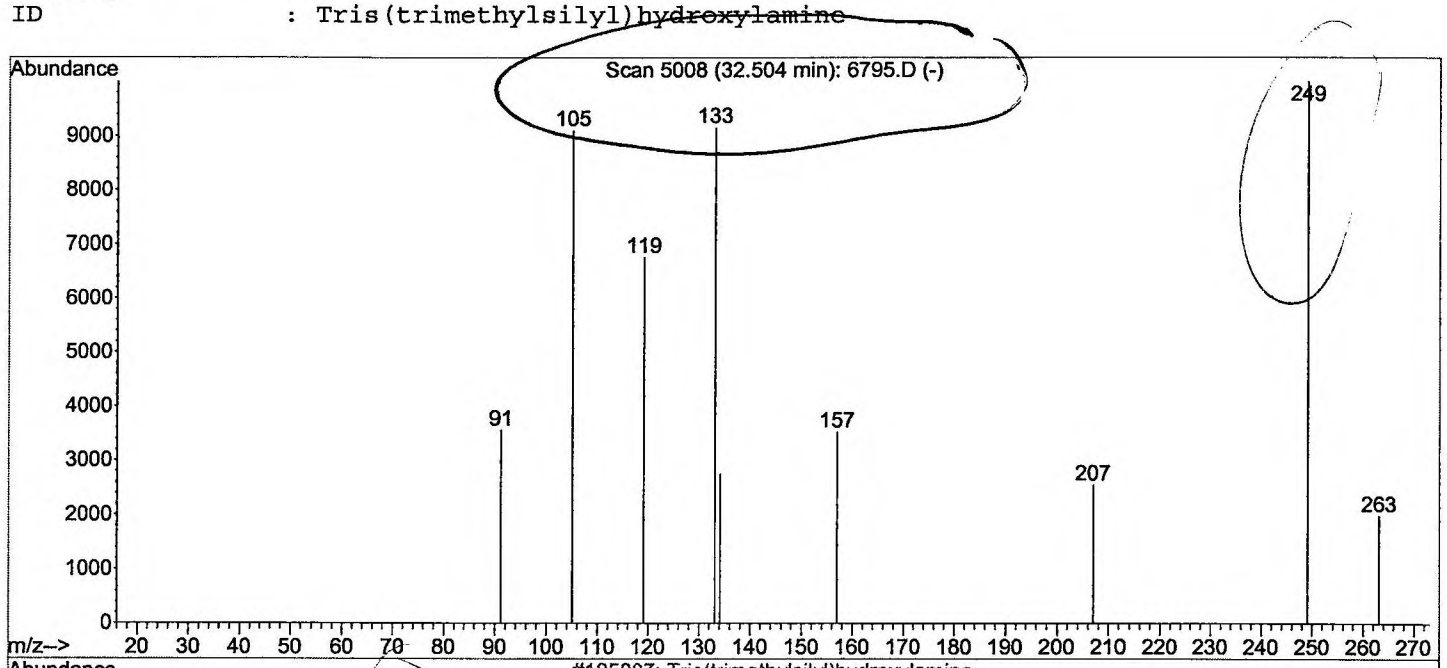
Library Searched : C:\Database\wiley7n.l
Quality : 4
ID : Mandelonitrile $$ Benzeneacetonitrile, .alpha.-hydroxy- (CAS) $$ Benzaldehyde, cyanohydrin $$ .alpha.-Cyanobenzyl alcohol $$ .alpha.-Hydroxybenzeneacetonitrile $$ Mandelic acid nitrile $$ Phenylglycolonitrile $$ Hydroxyphenylacetonitrile $$ Acetonitrile,

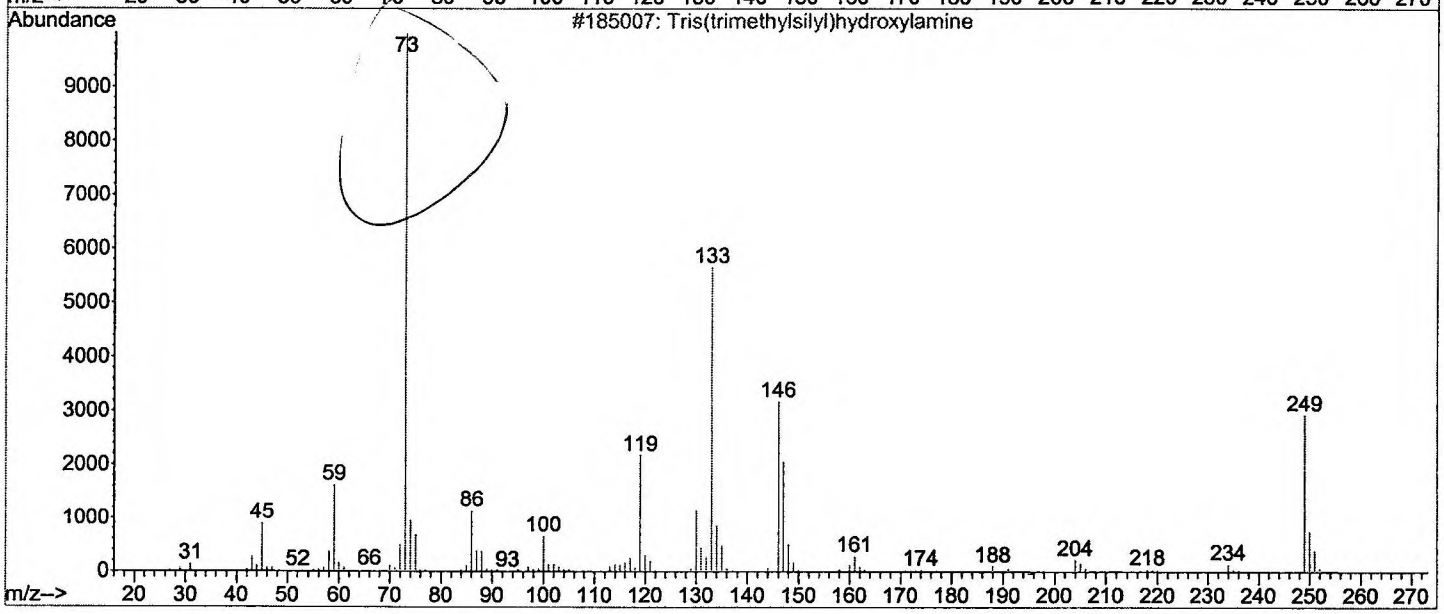


Library Searched : C:\Database\wiley7n.l
Quality : 4
ID : (3RS,3aRS,9aSR,9bRS)-1,3,3a,4,6,7,8,9,9a,9b-decahydro-6,6,9a-trimethylnaphtho[1,2-c]furan-3-ol $$ Naphtho[1,2-c]furan-3-ol, 1,3,3a,4,6,7,8,9,9a,9b-decahydro-6,6,9a-trimethyl-, (3.alpha.,3a.alpha.,9a.beta.,9b.alpha.)-(.+-.)- (CAS)

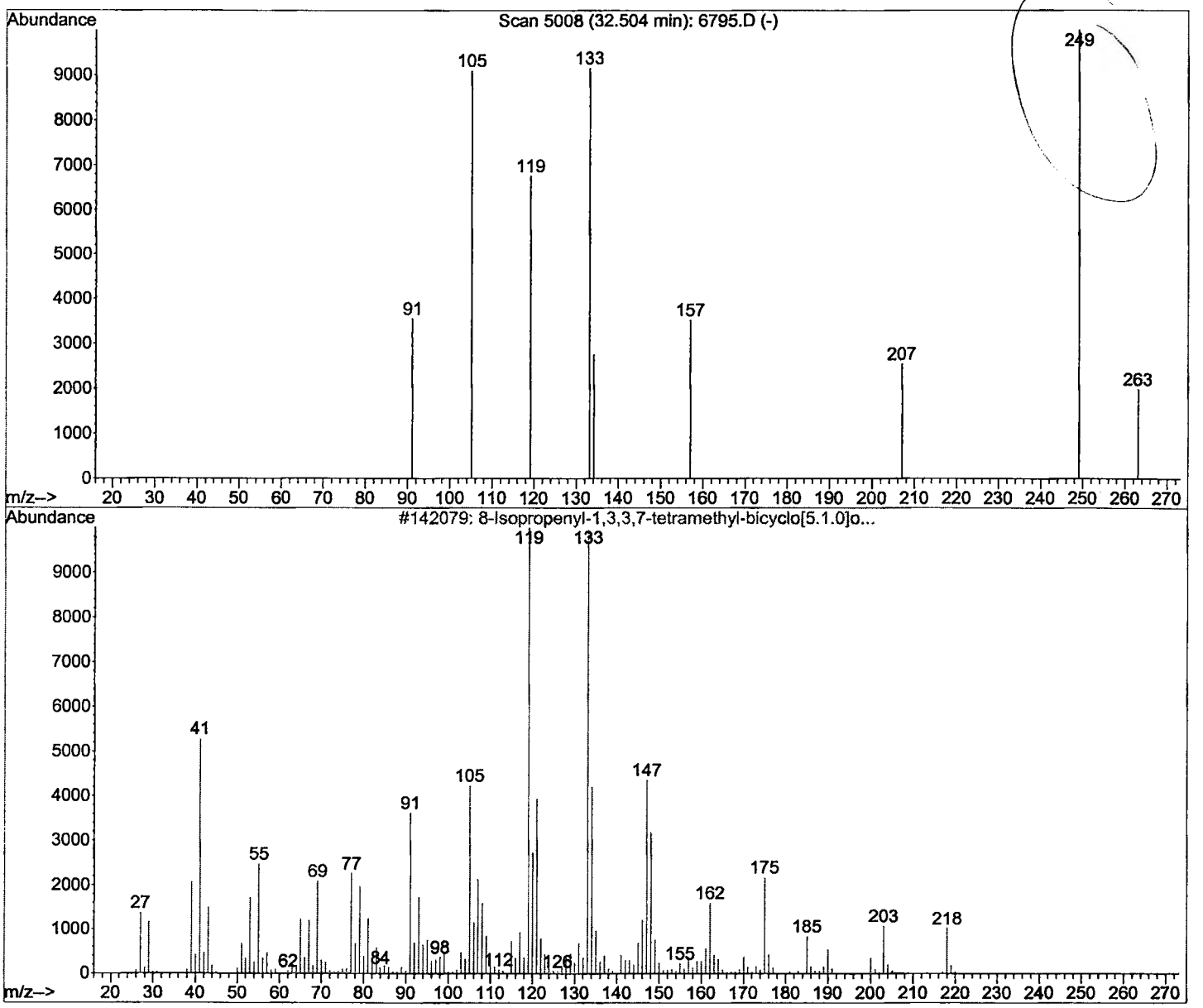


Library Searched : C:\Database\wiley7n.l
Quality : 9
ID : Tris(trimethylsilyl)hydroxylamine

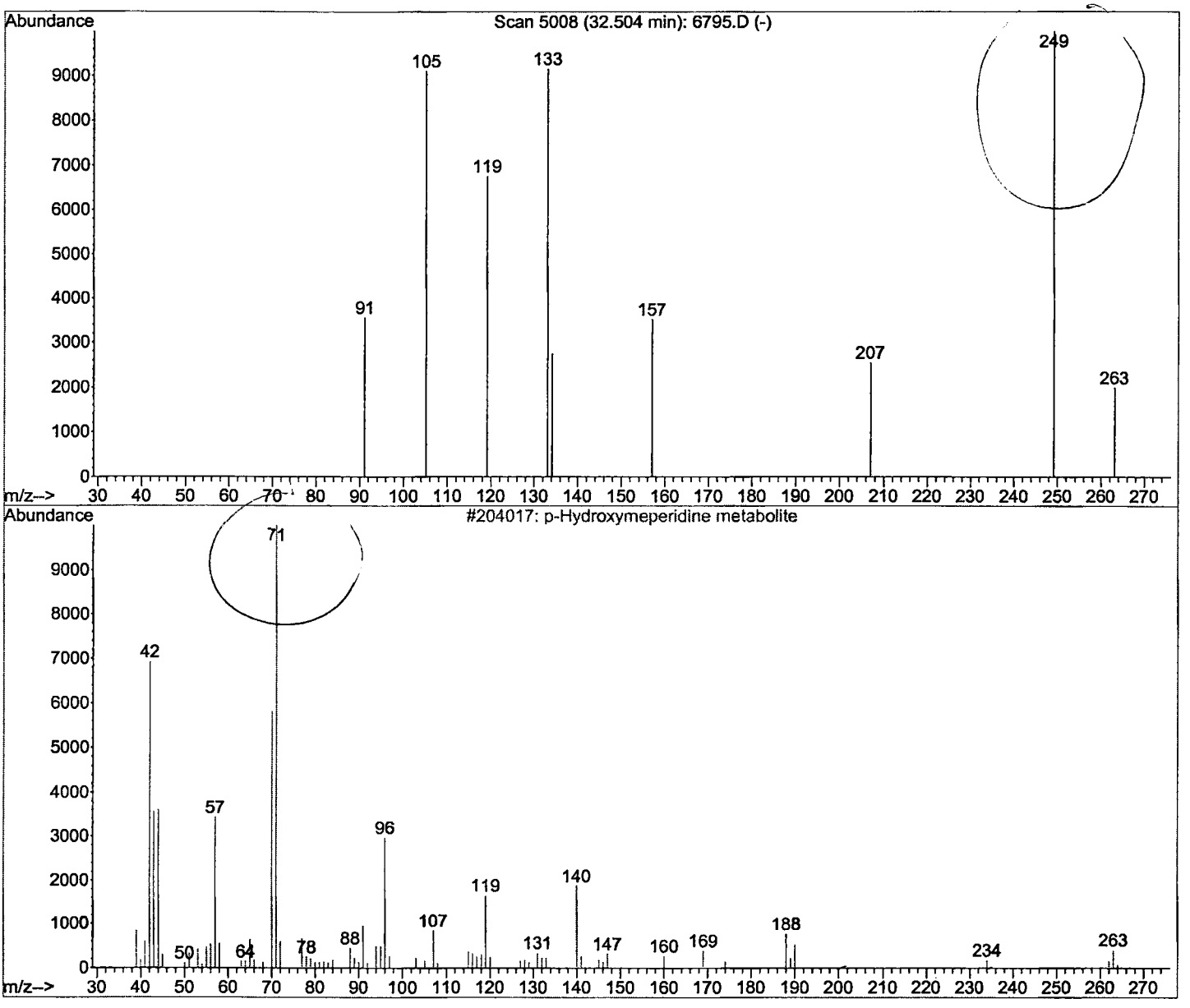




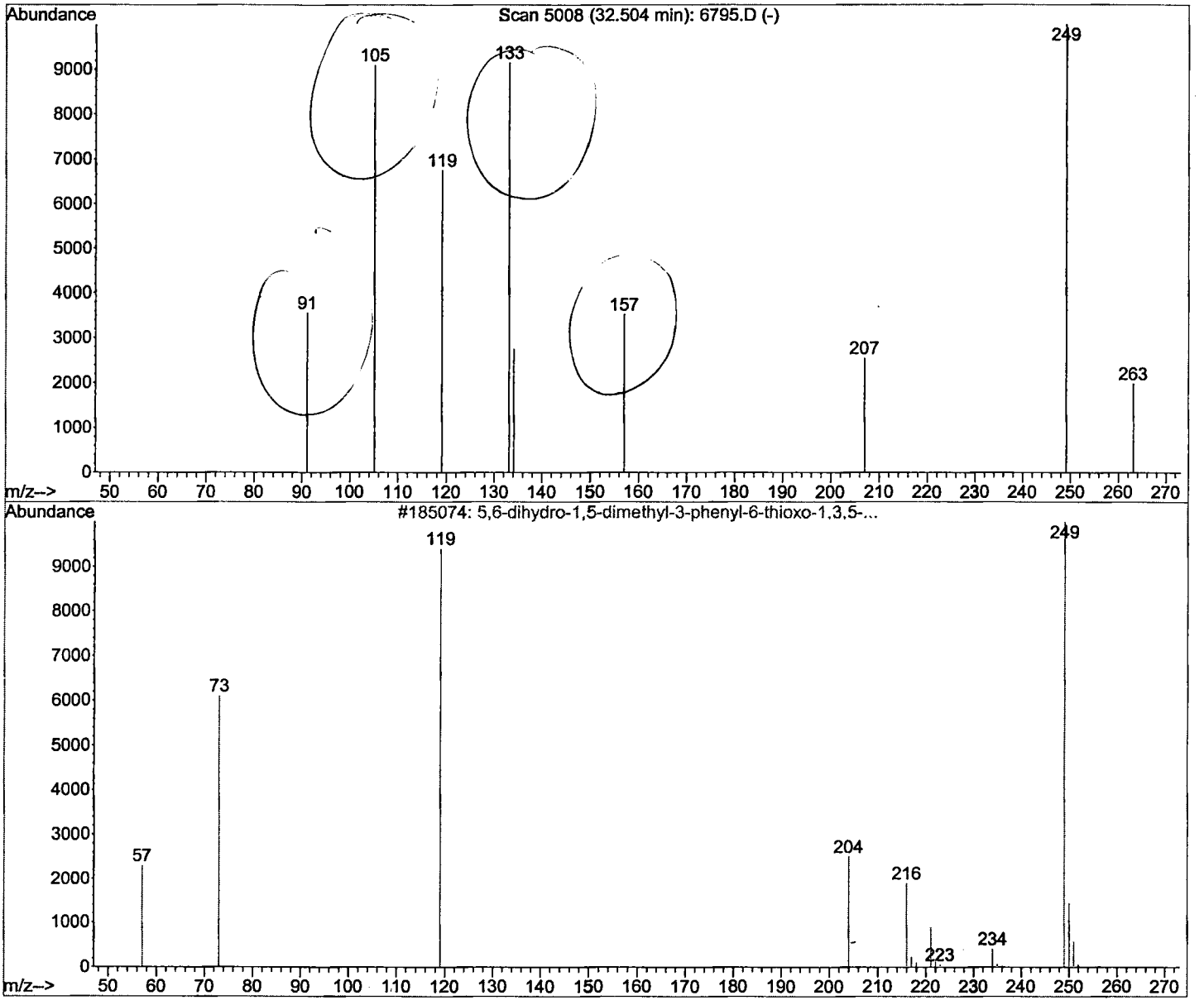
Library Searched : C:\Database\wiley7n.l
Quality : 9
ID : 8-Isopropenyl-1,3,3,7-tetramethyl-bicyclo[5.1.0]oct-5-en-2-one



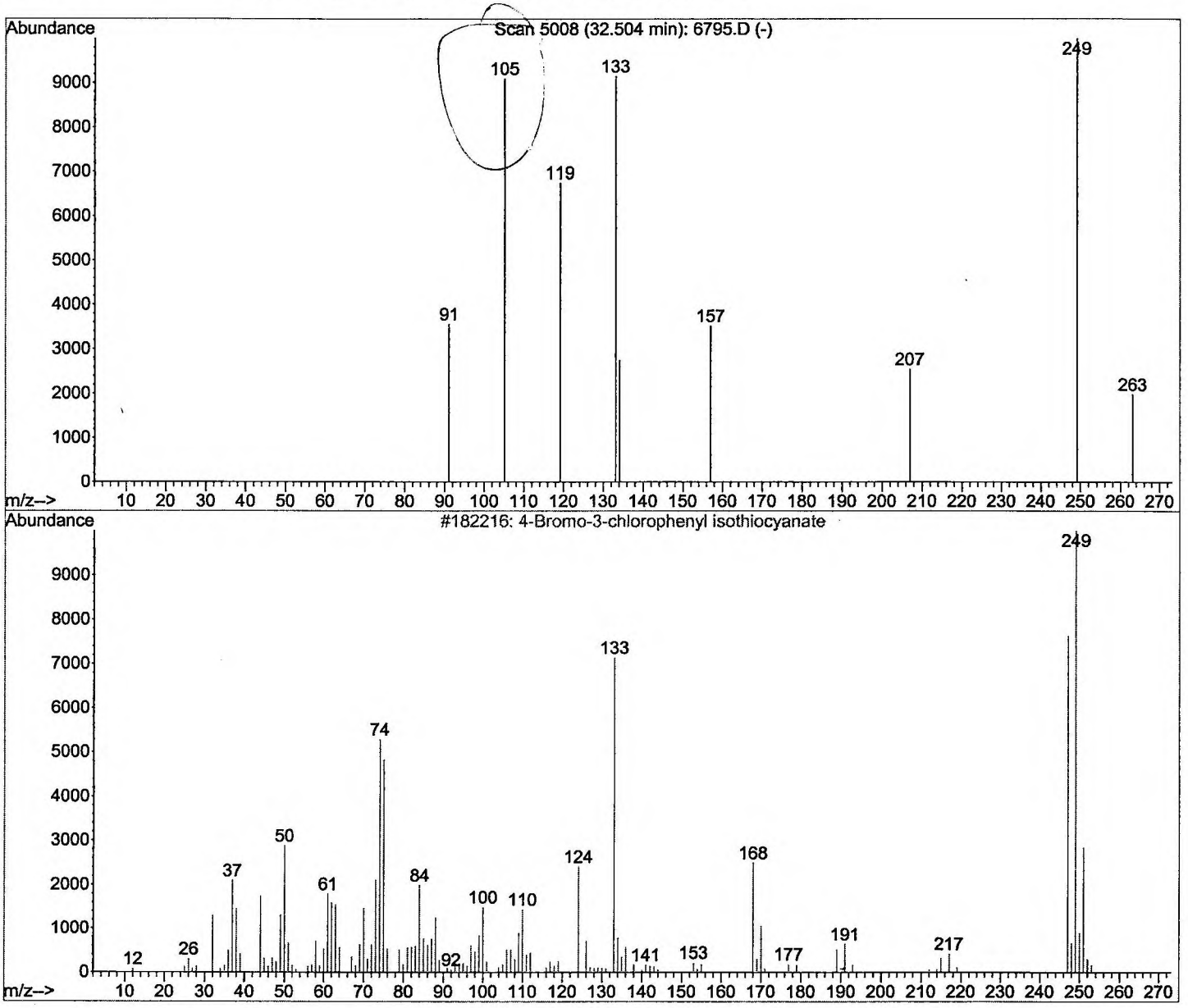
Library Searched : C:\Database\wiley7n.l
Quality : 7
ID : p-Hydroxymeperidine metabolite



Library Searched : C:\Database\wiley7n.l
Quality : 7
ID : 5,6-dihydro-1,5-dimethyl-3-phenyl-6-thioxo-1,3,5-triazine-2,4(1H,3H)-dione



Library Searched : C:\Database\wiley7n.l
Quality : 5
ID : 4-Bromo-3-chlorophenyl isothiocyanate



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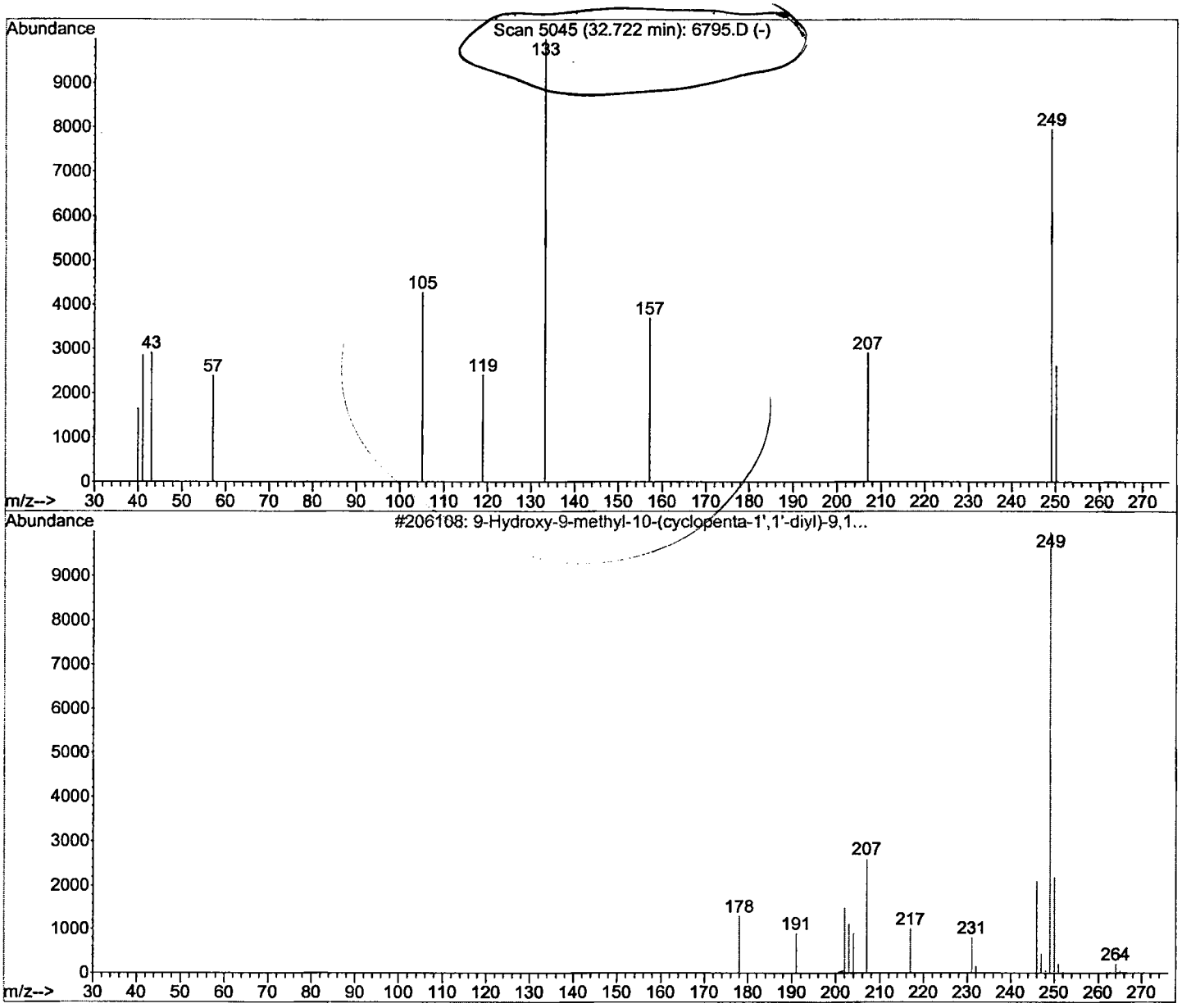
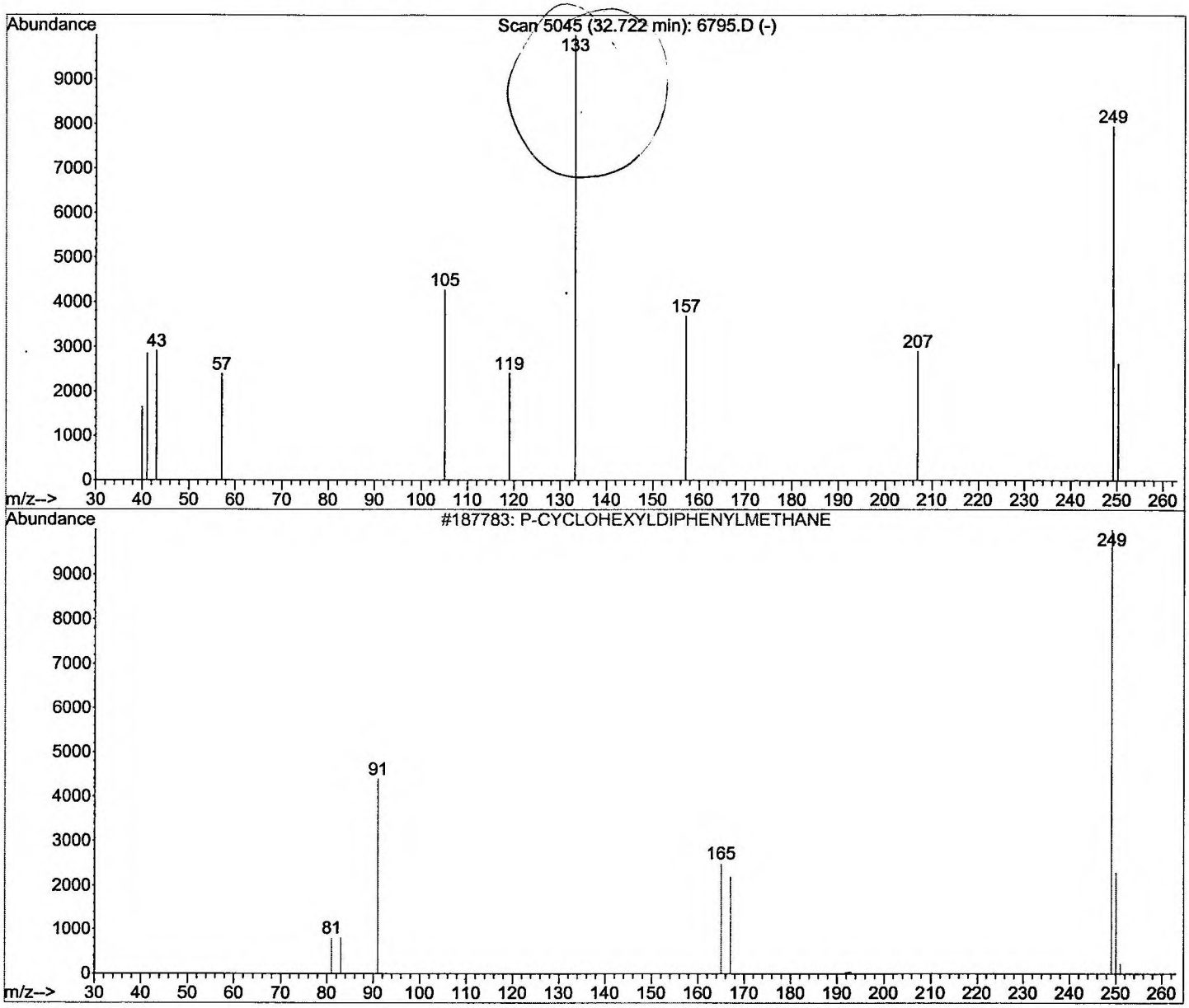
Quality : 9
ID : 9-Hydroxy-9-methyl-10-(cyclopenta-1',1'-diyl)-9,10-dihydroanthracene



Library Searched : C:\Database\wiley7n.l
Quality : 5
ID : P-CYCLOHEXYLDIPHENYLMETHANE



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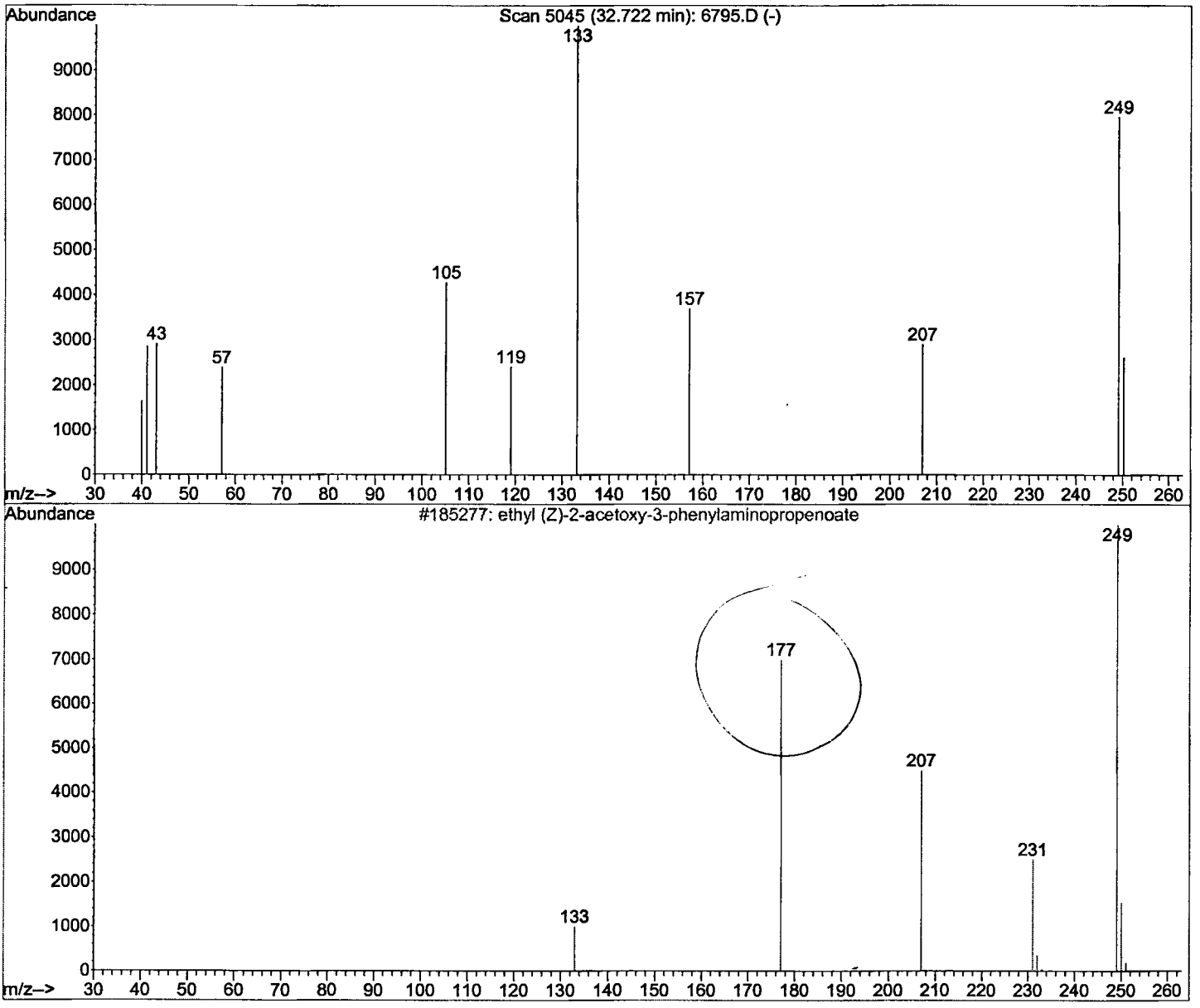
Quality : 5
ID : ethyl (Z)-2-acetoxy-3-phenylaminopropenoate



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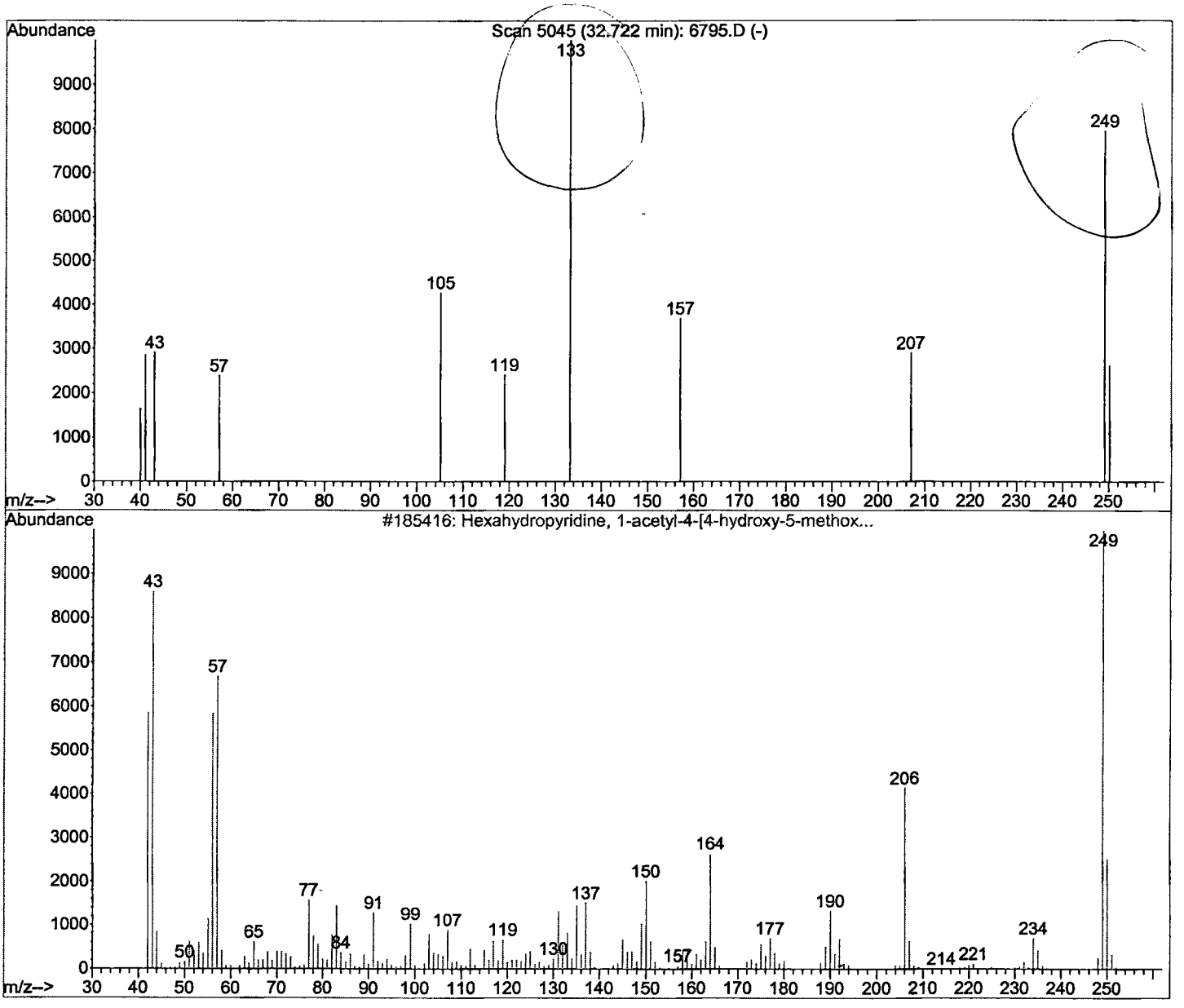
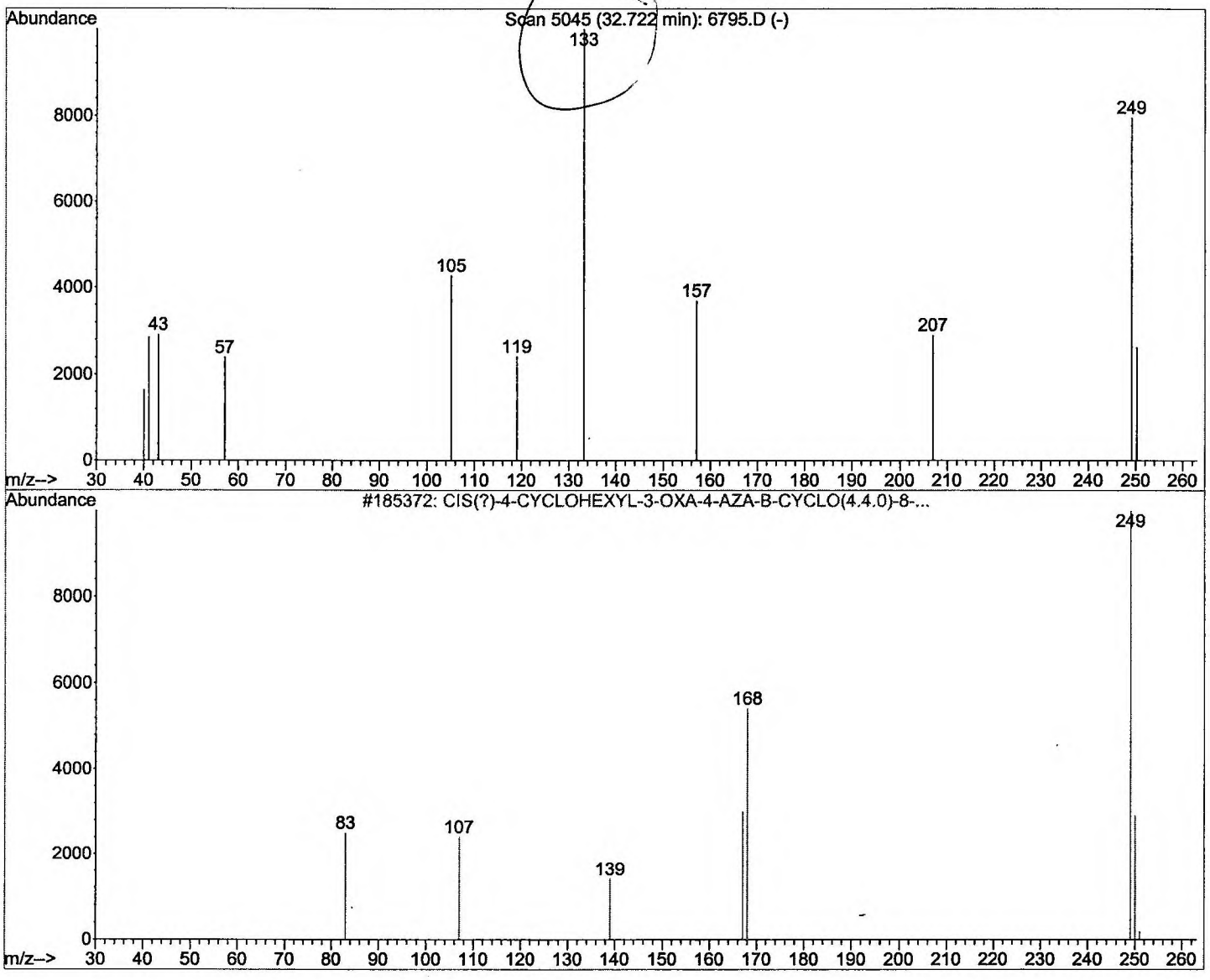
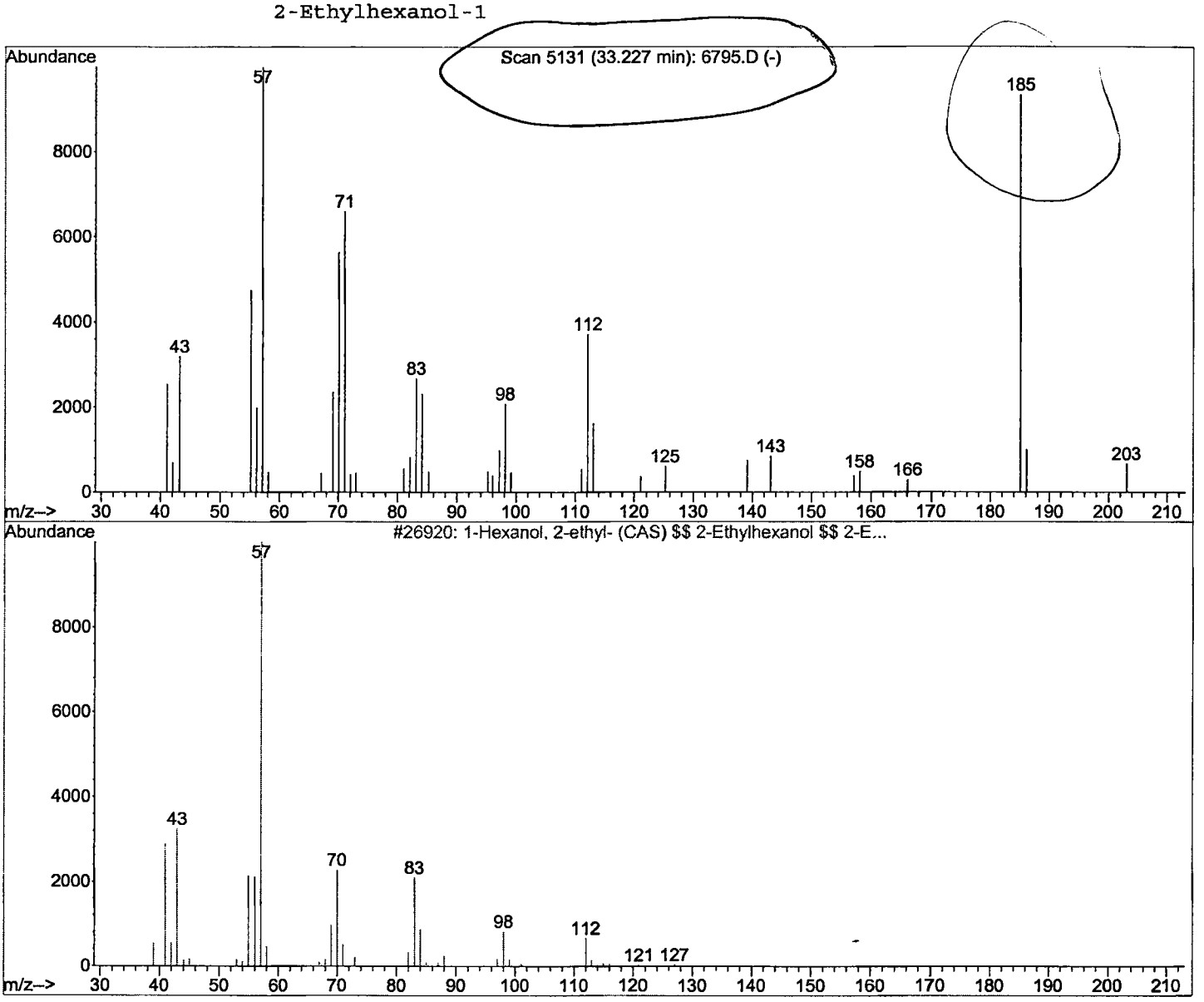
Quality : 5
ID : Hexahydropyridine, 1-acetyl-4-[4-hydroxy-5-methoxyphenyl]-



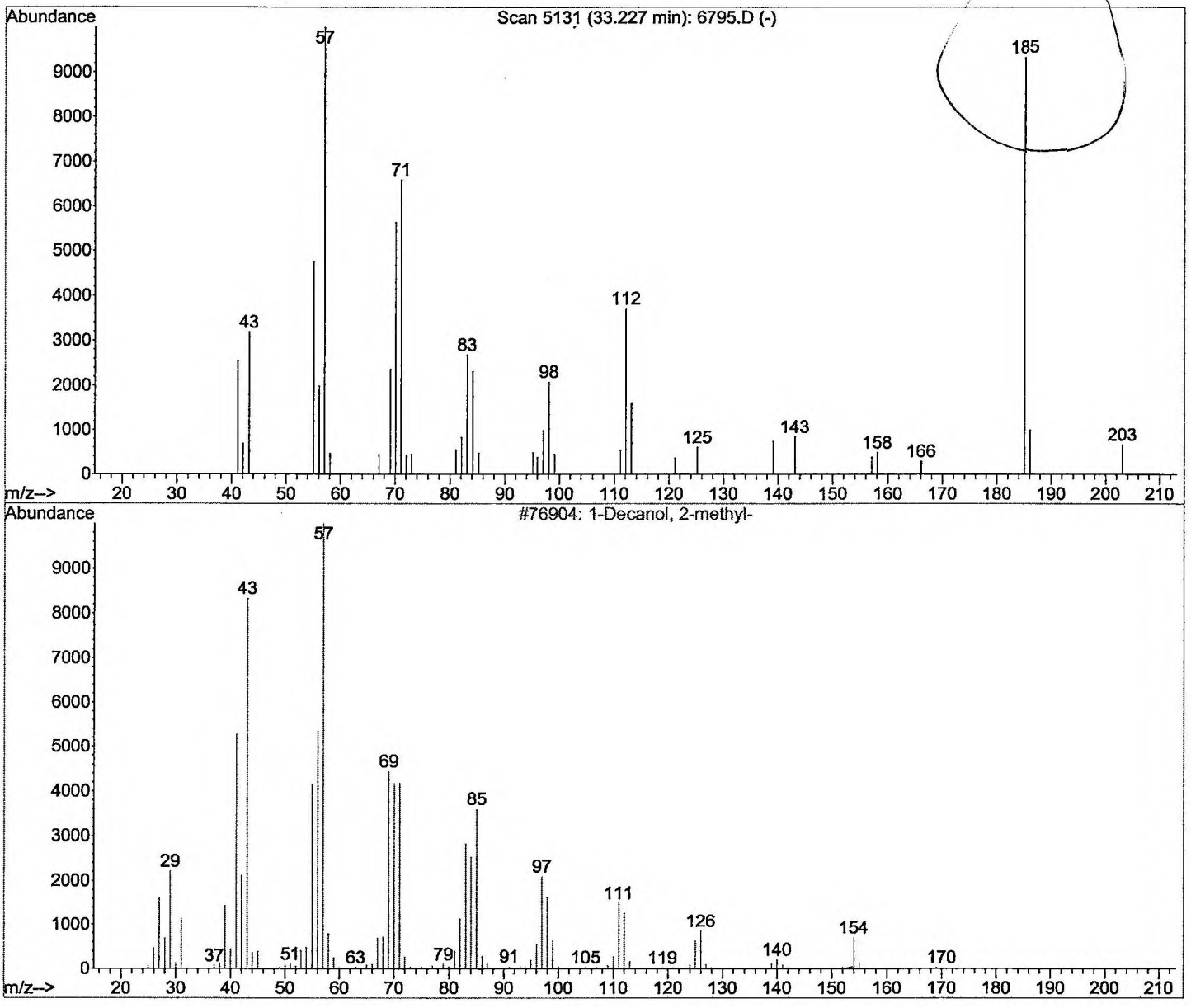
Library Searched : C:\Database\wiley7n.l
Quality : 5
ID : CIS(?)-4-CYCLOHEXYL-3-OXA-4-AZA-B-CYCLO(4.4.0)-8-DECEN-2,5-DIONE $$ 1H-2,3-Benzoxazine-1,4(3H)-dione, 3-cyclohexyl-4a,5,8,8a-tetrahydro-, cis- (CAS) $$ 3-Cyclohexyl-4a,5,8,8a-tetrahydrobenzo[d][1,2]oxazine-1,4-dione $$ 3-CYCLOHEXYL-4A,5,8,8A-TETRAHYDRO-BE



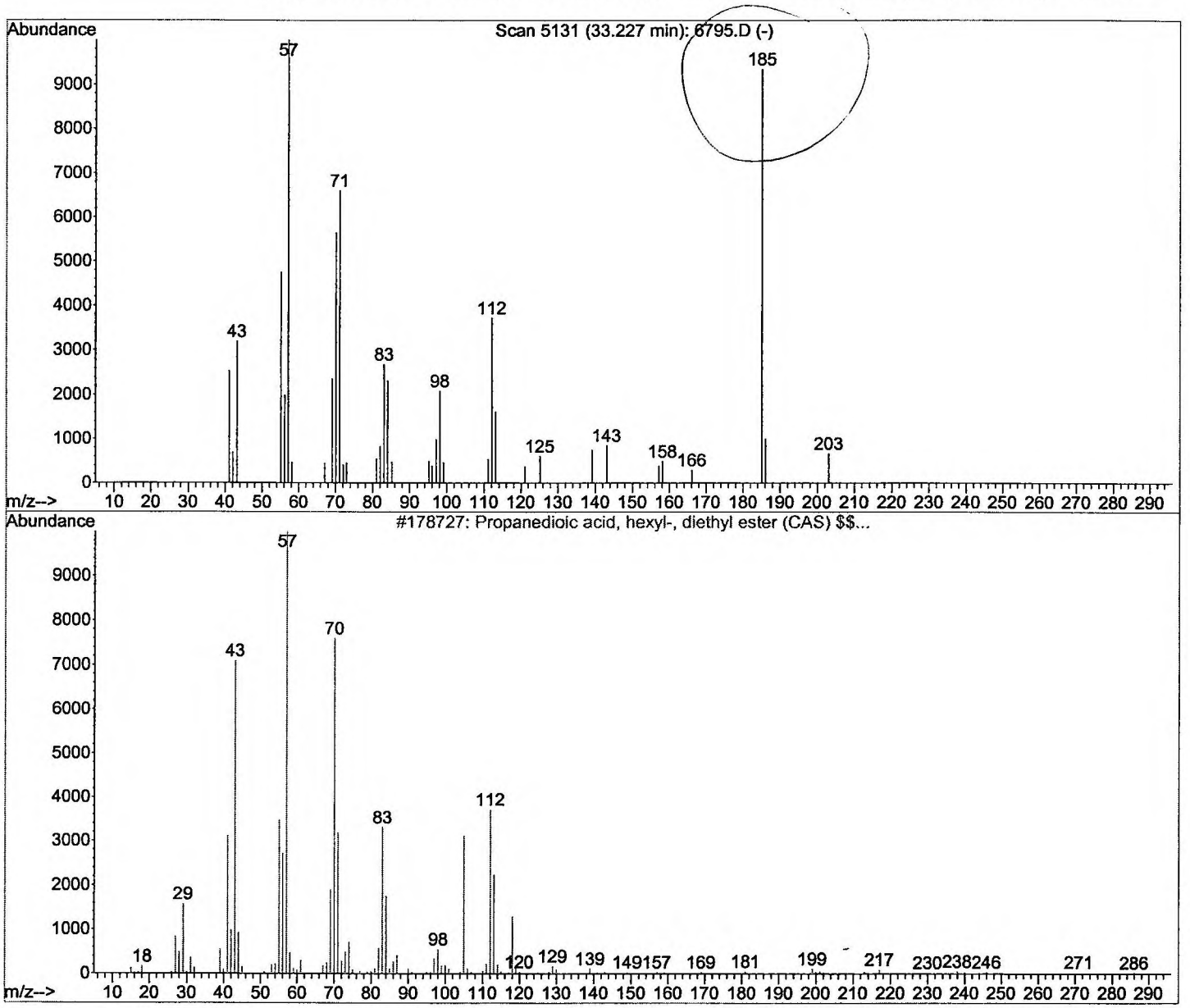
Library Searched : C:\Database\wiley7n.l
Quality : 38
ID : 1-Hexanol, 2-ethyl- (CAS) $$ 2-Ethylhexanol $$ 2-Ethyl-1-hexanol $$ Ethylhexanol $$ 2-Ethylhexan-1-ol $$ 2-Ethylhexyl alcohol $$ 2-Ethyl-hexanol-1 $$ Ethylhexyl alcohol $$ Octyl alcohol $$ 2-ETHYL-HEXAN-1-OL $$ 2-Ethylhexanol-1



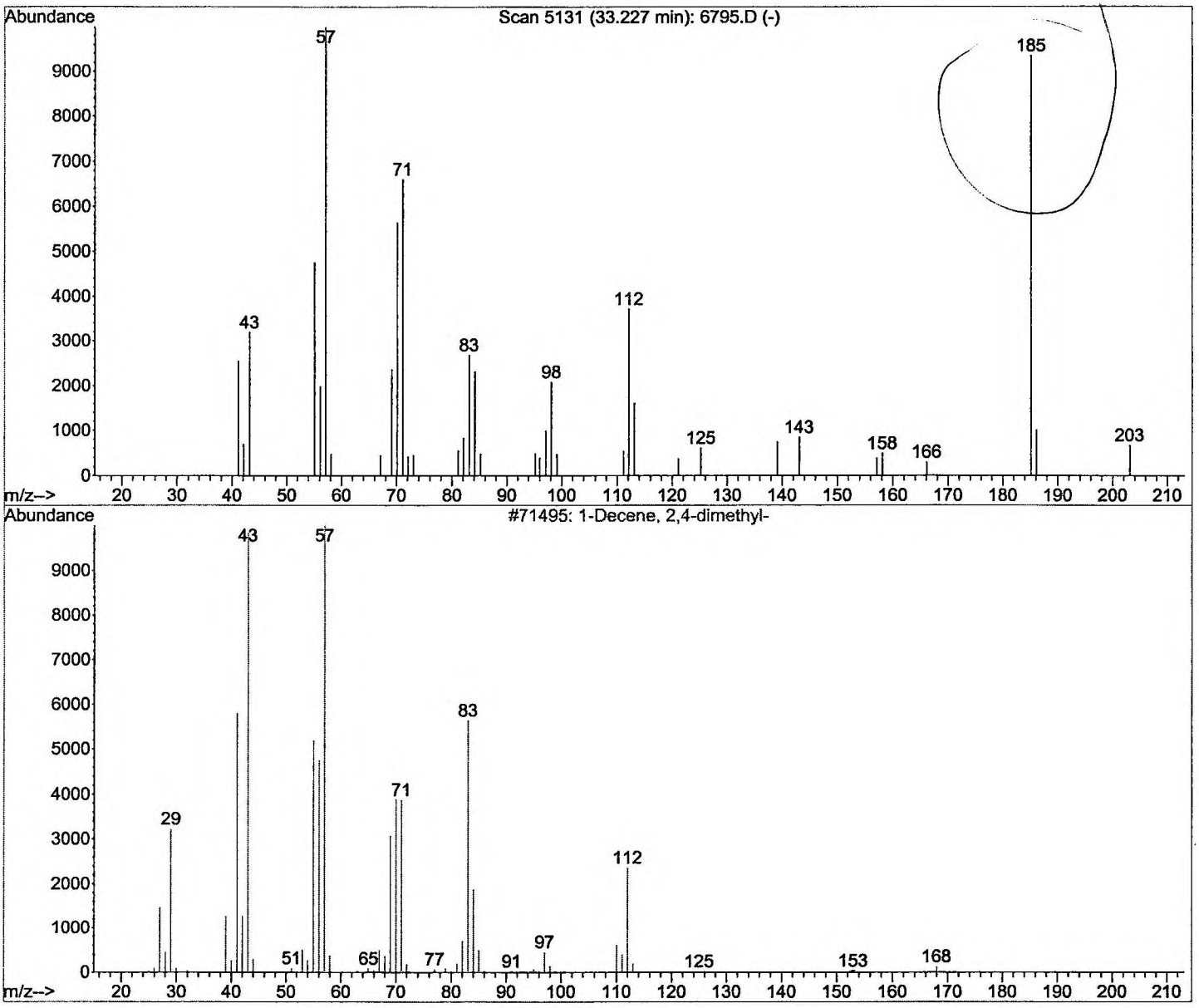
Library Searched : C:\Database\wiley7n.l
Quality : 37
ID : 1-Decanol, 2-methyl-



Library Searched : C:\Database\wiley7n.l
Quality : 35
ID : Propanedioic acid, hexyl-, diethyl ester (CAS) $$ Diethyl hexylmalonat
e $$ Diethyl 2-hexylmalonate $$ Malonic acid, hexyl-, diethyl ester



Library Searched : C:\Database\wiley7n.l
Quality : 35
ID : 1-Decene, 2,4-dimethyl-



Library Searched : C:\Database\wiley7n.l
Quality : 35
ID : DI(2-ETHYLHEXYL) MALONATE