

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111721\
 Data File : VY006798.D
 Acq On : 17 Nov 2021 19:49
 Operator : SY/MD
 Sample : M4695-03
 Misc : 5.08G/5ML/MSVOA_Y/SOIL
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 289

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
 Title : SW846 8260

Signal : TIC: VY006798.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.954	341	350	363	rVB	12345	33777	5.57%	0.878%
2	4.210	383	392	402	rBV2	4968	15639	2.58%	0.406%
3	4.722	465	476	490	rVB2	15138	46992	7.74%	1.221%
4	5.752	637	645	656	rBV6	2964	9157	1.51%	0.238%
5	6.996	838	849	870	rBV	21325	98563	16.24%	2.562%
6	7.728	959	969	974	rBV2	78014	186521	30.74%	4.848%
7	7.795	974	980	996	rVB	147271	328195	54.09%	8.530%
8	8.142	1024	1037	1050	rVB2	95600	261184	43.04%	6.789%
9	8.697	1119	1128	1137	rBV	229544	444051	73.18%	11.542%
10	9.081	1184	1191	1198	rBV2	14296	28976	4.78%	0.753%
11	10.185	1364	1372	1380	rBV	353179	606803	100.00%	15.772%
12	10.581	1429	1437	1450	rVB	27609	48722	8.03%	1.266%
13	10.953	1492	1498	1510	rBV	24695	51149	8.43%	1.329%
14	11.319	1551	1558	1566	rVB	28563	48241	7.95%	1.254%
15	11.489	1579	1586	1596	rBV	300149	495626	81.68%	12.882%
16	12.337	1719	1725	1733	rBV	37984	59640	9.83%	1.550%
17	12.483	1742	1749	1757	rBV2	286432	511048	84.22%	13.283%
18	12.830	1796	1806	1813	rBV7	3505	9249	1.52%	0.240%
19	13.148	1851	1858	1861	rBV	21913	35702	5.88%	0.928%
20	13.184	1861	1864	1869	rVB	9927	14251	2.35%	0.370%
21	13.428	1896	1904	1911	rBV	236316	368856	60.79%	9.587%
22	13.964	1986	1992	2003	rVB	24076	43178	7.12%	1.122%
23	14.257	2034	2040	2045	rBV8	7944	15466	2.55%	0.402%
24	14.422	2063	2067	2071	rBV6	6058	8551	1.41%	0.222%
25	14.623	2095	2100	2104	rBV6	4041	7936	1.31%	0.206%
26	14.684	2104	2110	2114	rBV5	6353	11232	1.85%	0.292%
27	14.739	2114	2119	2125	rVB8	5737	9640	1.59%	0.251%
28	14.934	2149	2151	2156	rVB6	4044	6362	1.05%	0.165%
29	15.123	2178	2182	2186	rBV7	4546	6302	1.04%	0.164%
30	15.281	2202	2208	2211	rBV8	4464	10871	1.79%	0.283%
31	15.610	2257	2262	2266	rVB5	7105	13017	2.15%	0.338%
32	16.482	2401	2405	2412	rVB10	5470	12522	2.06%	0.325%

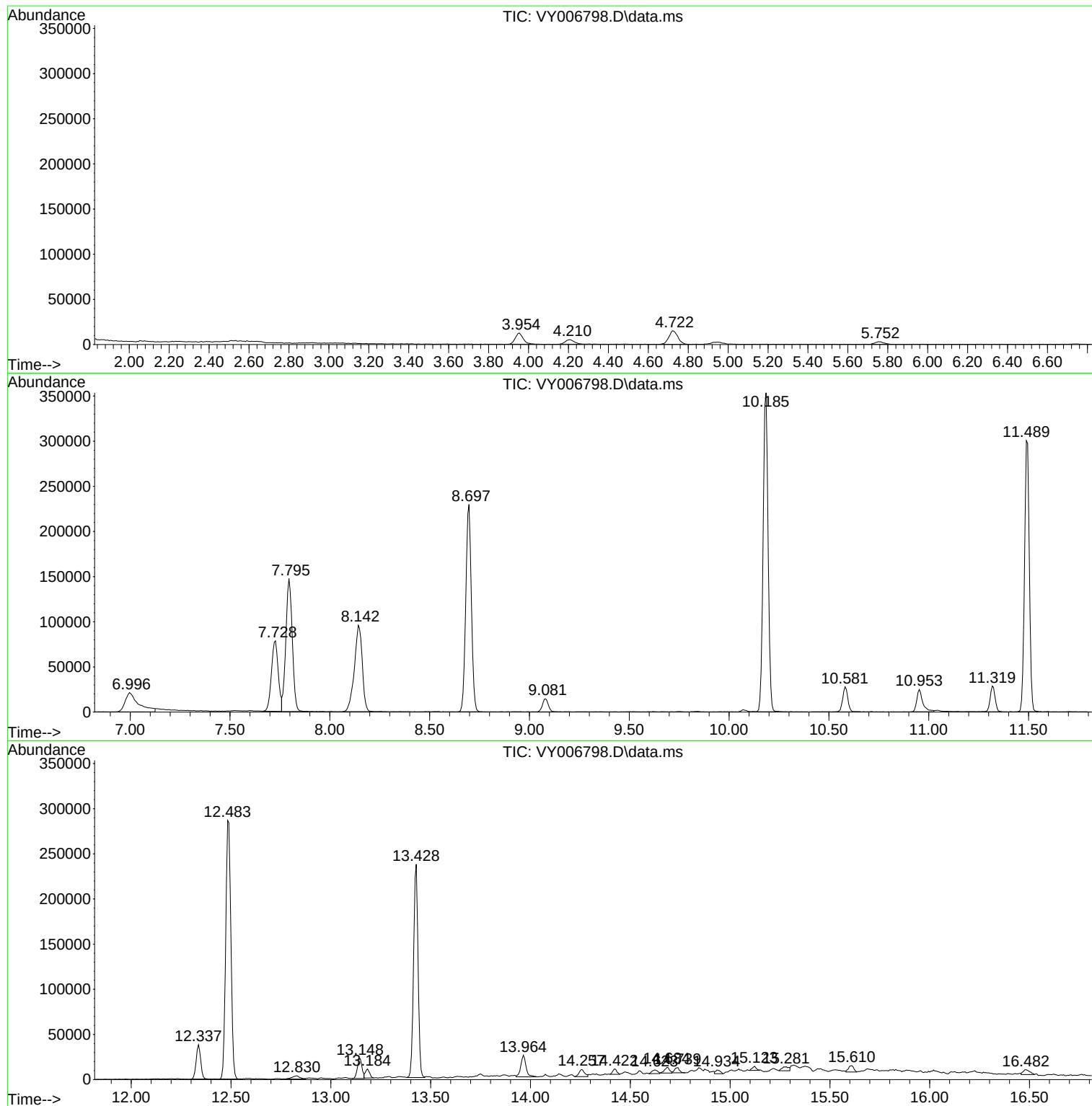
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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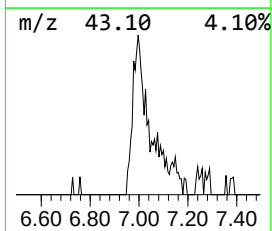
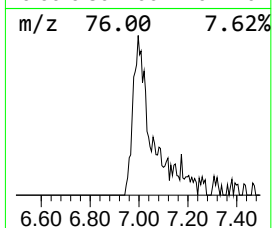
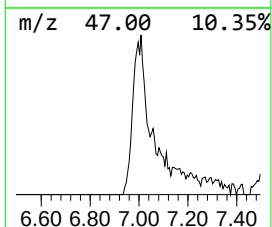
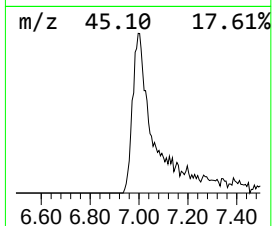
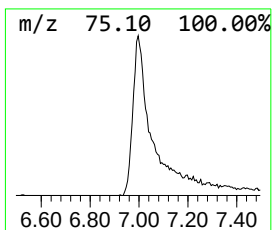
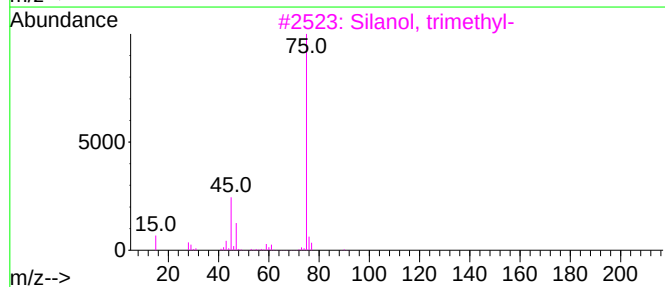
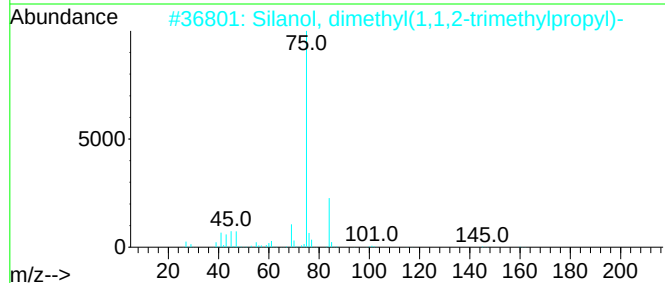
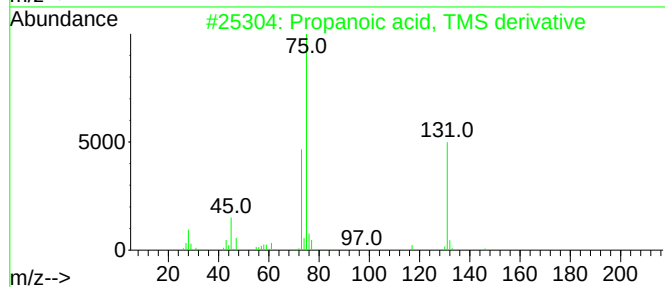
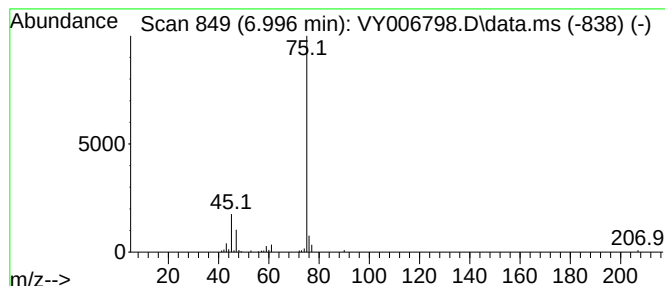
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, TMS derivative Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.996	15.02 ug/l	98563	Pentafluorobenzene	7.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	78
2			Silanol, dimethyl(1,1,2-trimethyl...	160	C8H20OSi	055644-10-5	78
3			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	78
4			Acetic acid, TMS derivative	132	C5H12O2Si	002754-27-0	64
5			Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	50



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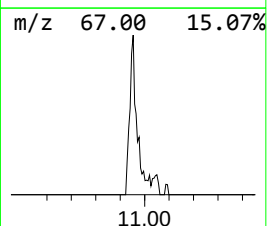
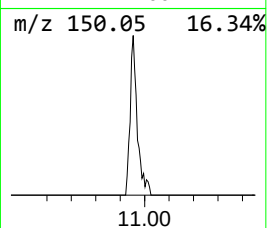
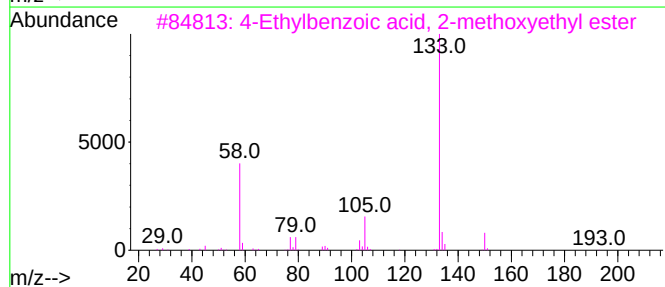
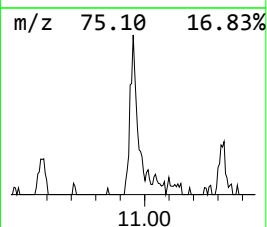
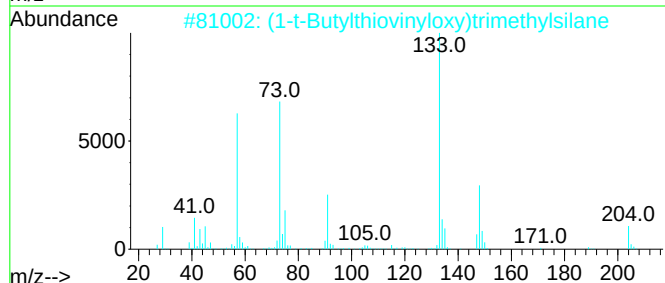
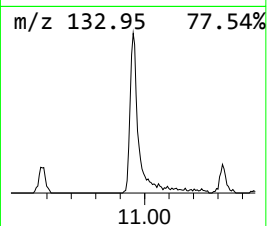
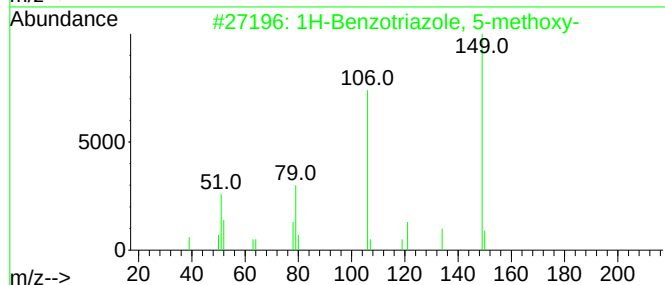
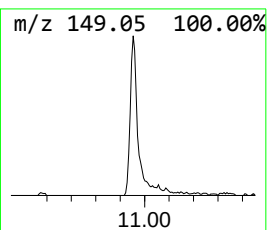
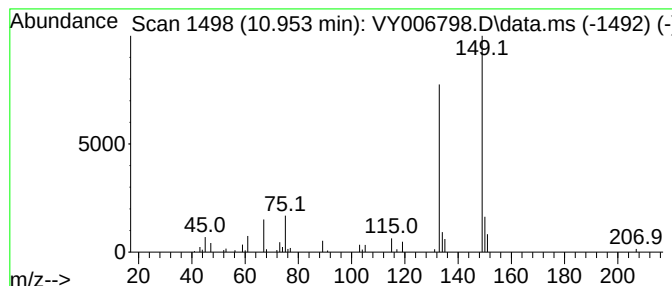
Instrument :
MSVOA_Y
ClientSampleId :
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Quant Title : SW846 8260

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Peak Number 3 unknown10.953 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.953	5.16 ug/l	51149	Chlorobenzene-d5	11.495	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	25
2	(1-t-Butylthiovinloxy)trimethyl...	204	C9H20OSSi	063584-47-4	25
3	4-Ethylbenzoic acid, 2-methoxyet...	208	C12H16O3	1000331-30-6	17
4	4-Ethylbenzoic acid, 2-methylbut...	220	C14H20O2	1000331-30-8	17
5	4-Ethylbenzoic acid, cyclohexyl ...	232	C15H20O2	1000293-32-1	17



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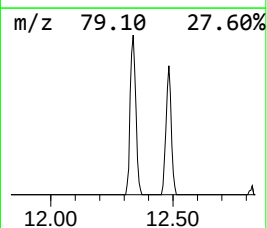
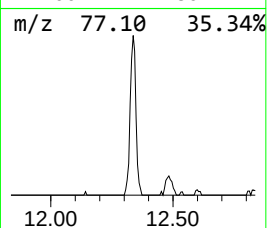
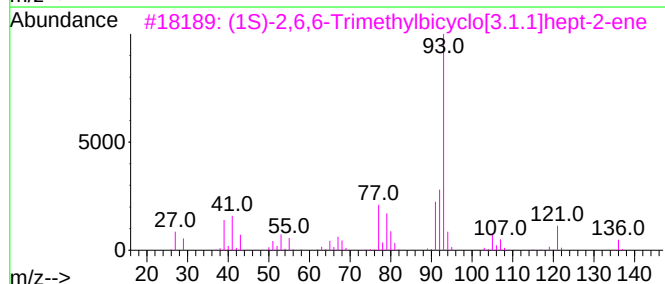
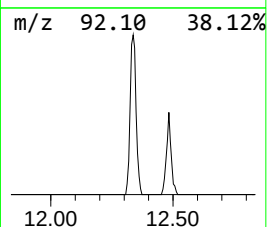
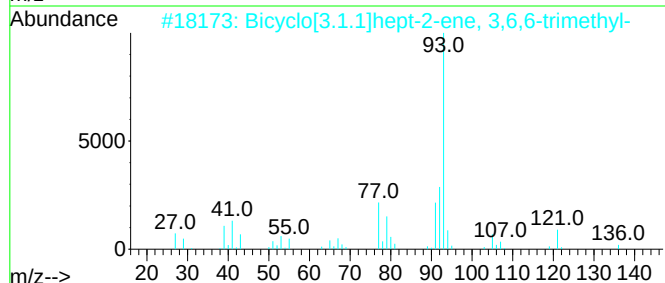
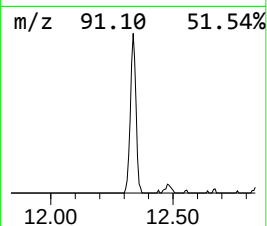
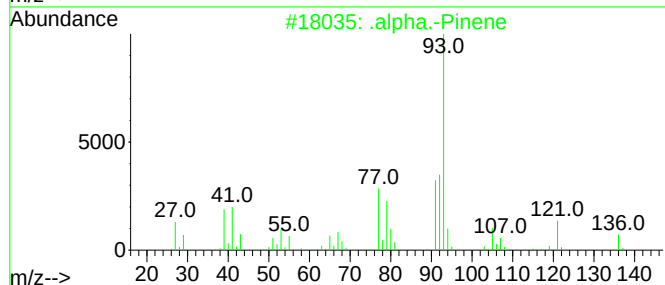
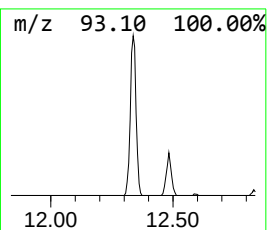
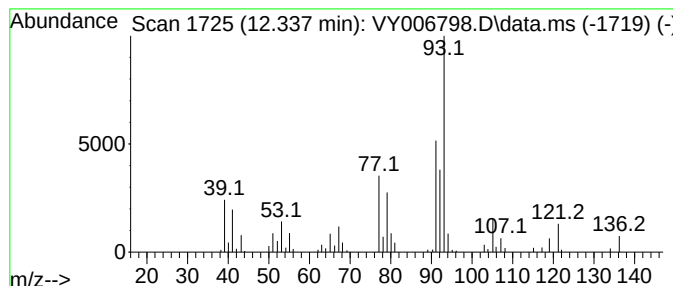
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Peak Number 4 .alpha.-Pinene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.337	6.02 ug/l	59640	Chlorobenzene-d5	11.495	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Pinene	136	C10H16	000080-56-8	97
2	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
3	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	90
4	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	87
5	.gamma.-Terpinene	136	C10H16	000099-85-4	80



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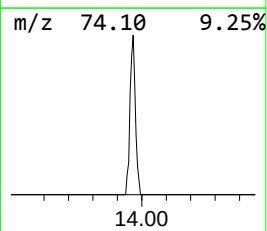
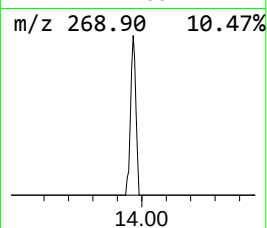
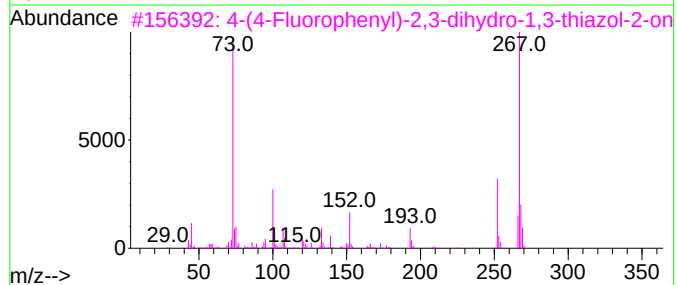
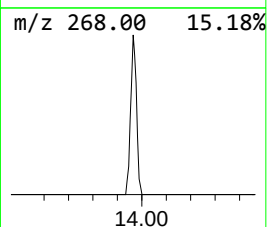
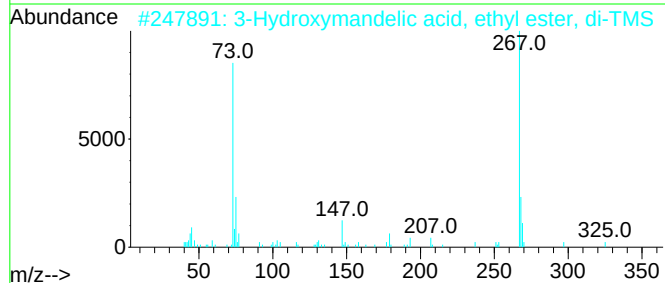
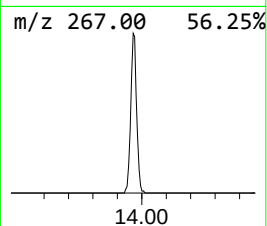
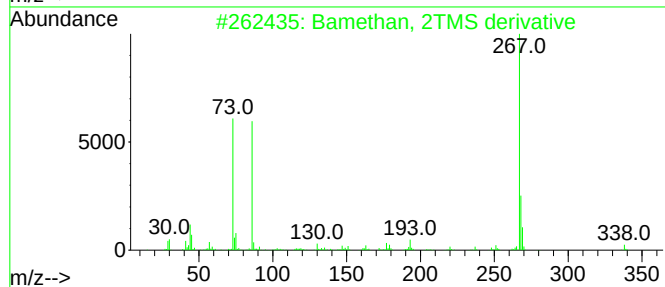
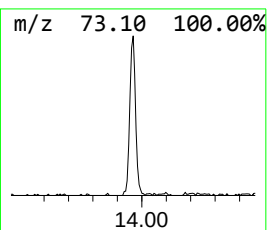
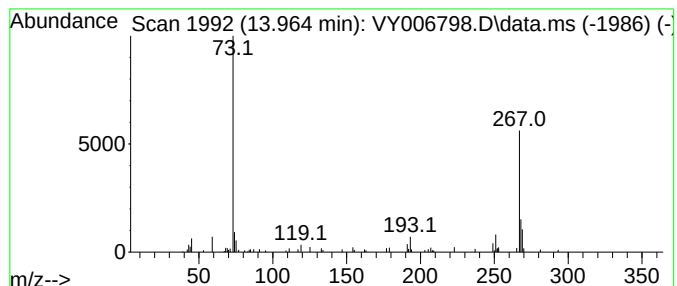
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Bamethan, 2TMS derivative Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.964	5.85 ug/l	43178	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	72
2			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	64
3			4-(4-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSi	1010501-61-0	64
4			4-(2-amino-1-hydroxypropyl)pheno...	311	C15H29NO2Si2	1000478-98-6	64
5			9-Acridinol, trimethylsilyl ether	267	C16H17NOSi	1000463-65-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	6.996	15.0	ug/l	98563	1	7.795	328195	50.0
unknown10.953	10.953	5.2	ug/l	51149	3	11.495	495626	50.0
.alpha.-Pinene	12.337	6.0	ug/l	59640	3	11.495	495626	50.0
Bamethan, 2TMS ...	13.964	5.8	ug/l	43178	4	13.428	368856	50.0