

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY111521\
 Data File : VY006743.D
 Acq On : 15 Nov 2021 20:09
 Operator : SY/MD
 Sample : M4680-02
 Misc : 5.83G/5ML/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 COMP-2

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: VY006743.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.509	110	113	118	rBV4	1466	2478	1.51%	0.242%
2	4.735	469	478	485	rVB6	1727	4698	2.86%	0.459%
3	5.771	641	648	653	rBV4	911	2370	1.44%	0.232%
4	7.728	959	969	975	rBV2	23517	54955	33.47%	5.369%
5	7.801	975	981	992	rVB2	42488	95999	58.46%	9.380%
6	8.142	1024	1037	1047	rBV3	33443	106920	65.11%	10.447%
7	8.697	1119	1128	1136	rBV	65614	127569	77.69%	12.464%
8	9.081	1185	1191	1197	rBV3	2355	4738	2.89%	0.463%
9	10.185	1365	1372	1380	rBV	96132	164206	100.00%	16.044%
10	10.587	1430	1438	1443	rBV	9627	18962	11.55%	1.853%
11	10.959	1493	1499	1506	rVB2	989	1773	1.08%	0.173%
12	11.319	1553	1558	1566	rVB	7946	13271	8.08%	1.297%
13	11.496	1581	1587	1598	rBV	82437	132881	80.92%	12.983%
14	12.343	1720	1726	1734	rBV	8711	13395	8.16%	1.309%
15	12.489	1741	1750	1759	rBV2	80480	142583	86.83%	13.931%
16	13.074	1837	1846	1852	rBV6	1499	2764	1.68%	0.270%
17	13.148	1852	1858	1862	rVV3	5677	9244	5.63%	0.903%
18	13.184	1862	1864	1872	rVB	3078	4563	2.78%	0.446%
19	13.288	1872	1881	1886	rVB5	1895	4192	2.55%	0.410%
20	13.367	1889	1894	1898	rBV4	1148	1761	1.07%	0.172%
21	13.428	1898	1904	1910	rVV	65666	98914	60.24%	9.664%
22	13.483	1910	1913	1920	rVB3	1493	2916	1.78%	0.285%
23	13.648	1934	1940	1945	rVB6	1026	1746	1.06%	0.171%
24	13.971	1987	1993	1999	rBV	6667	10589	6.45%	1.035%

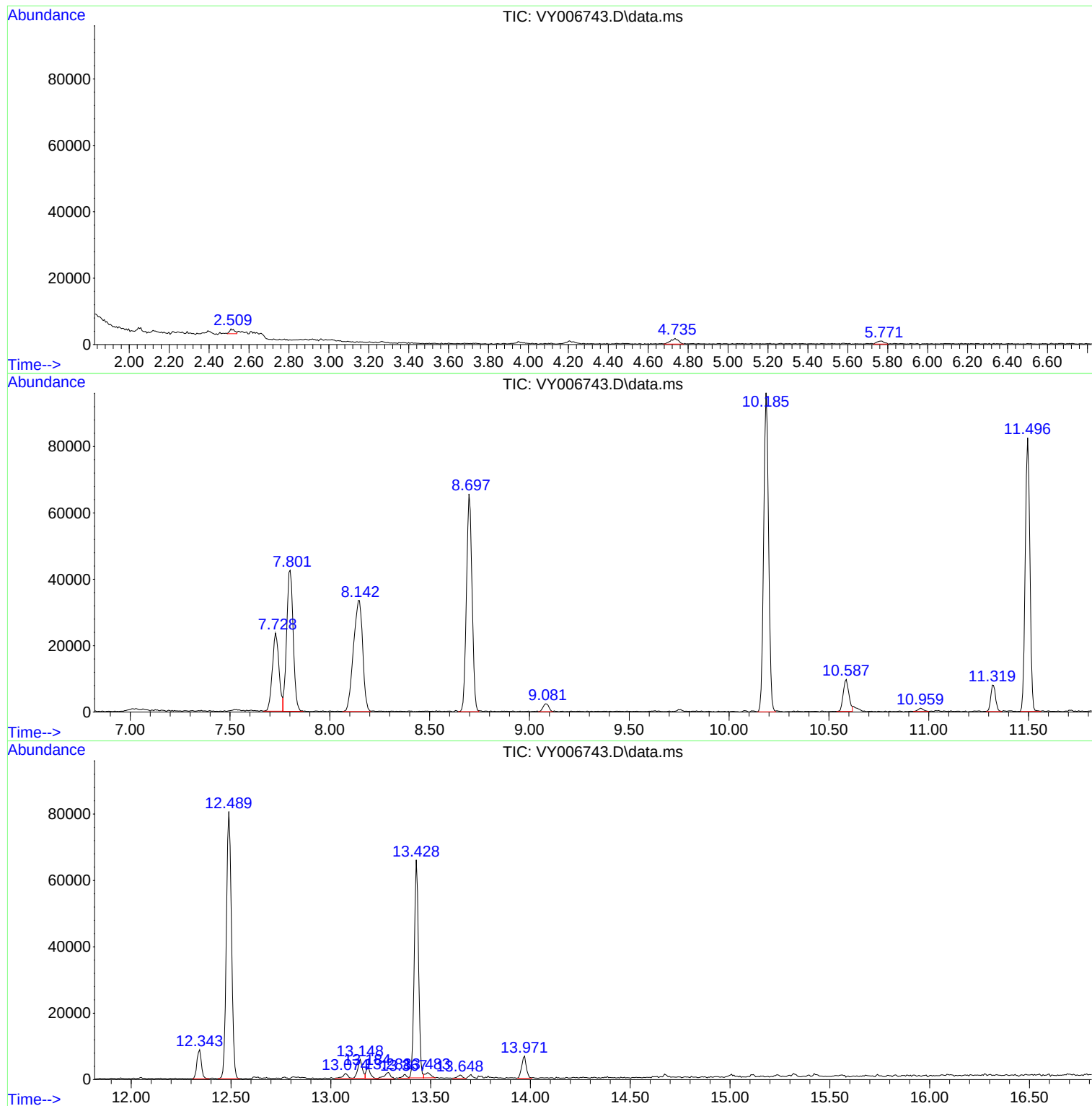
Sum of corrected areas: 1023487

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Quant Title : SW846 8260

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



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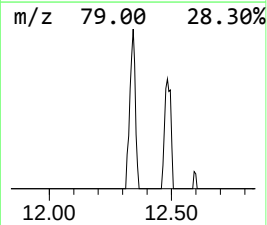
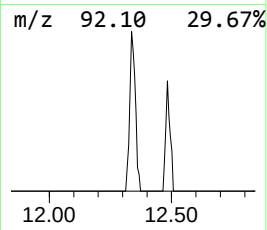
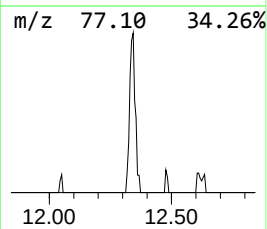
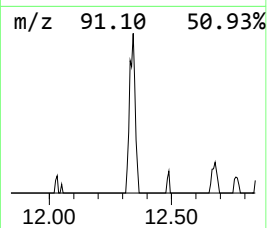
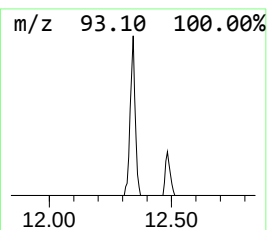
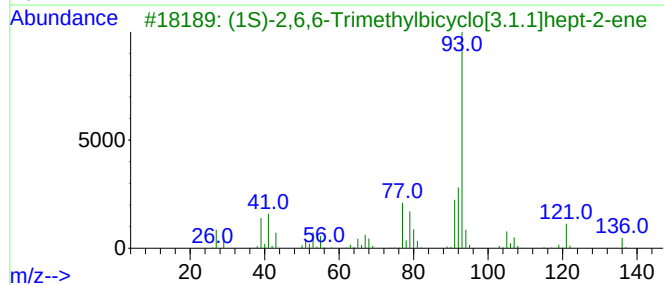
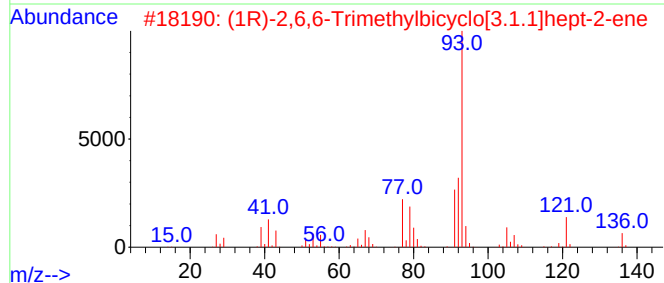
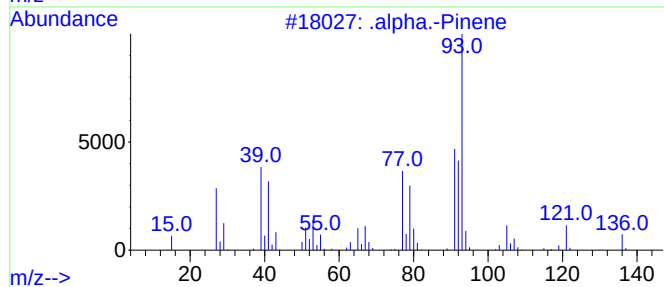
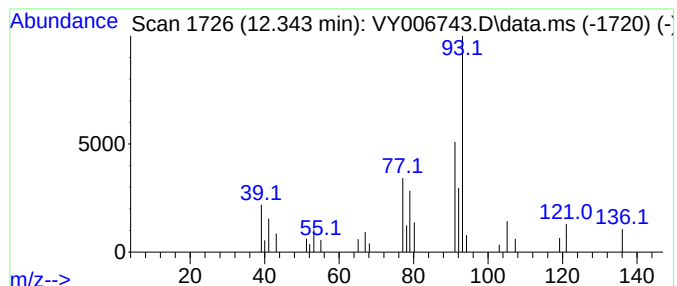
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y111521S.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 2 .alpha.-Pinene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.343	5.04 ug/l	13395	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Pinene	136	C10H16	000080-56-8	91
2			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	91
3			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	91
4			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	90



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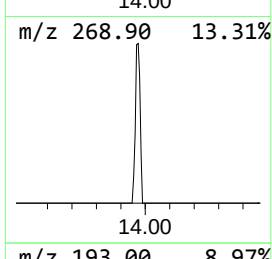
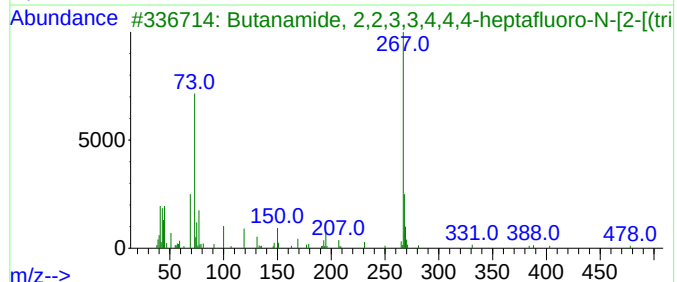
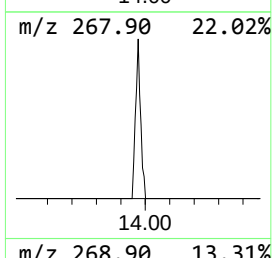
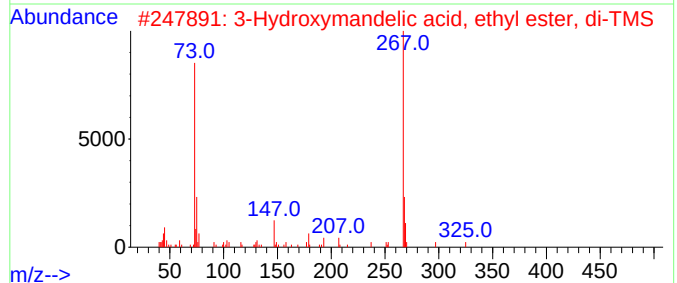
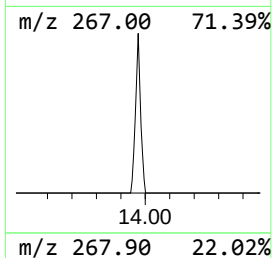
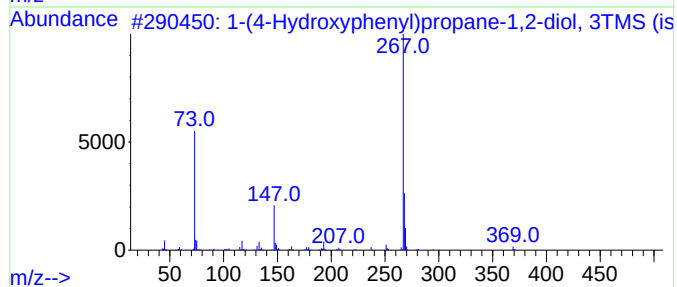
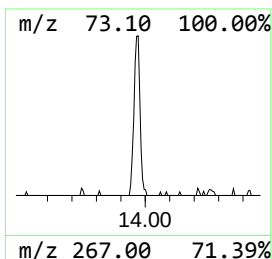
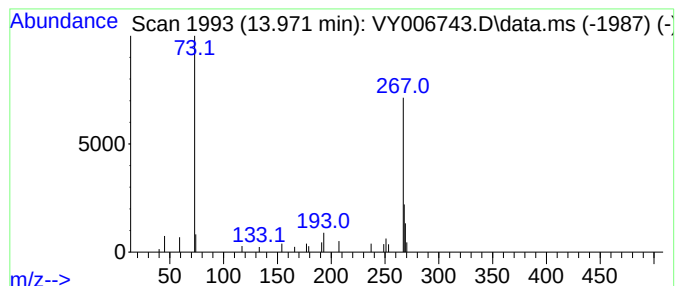
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Peak Number 3 1-(4-Hydroxyphenyl)propane-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.971	5.35 ug/l	10589	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Hydroxyphenyl)propane-1,2-d...	384	C18H36O3Si3	1000495-85-7	64
2			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	56
3			Butanamide, 2,2,3,3,4,4,4-hepta...	493	C18H26F7N3Si2	055471-01-7	50
4			Propenenitrile, 2-(2-benzothiazo...	268	C14H8N2S2	106833-31-2	49
5			6-Chloro-2,3-dimethyl-4-phenylqu...	267	C17H14ClN	022609-11-6	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
.alpha.-Pinene	12.343	5.0	ug/l	13395	3	11.496	132881	50.0
1-(4-Hydroxyphe...	13.971	5.3	ug/l	10589	4	13.428	98914	50.0