

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052620\
 Data File : VU038298.D
 Acq On : 26 May 2020 15:50
 Operator : JC/MD
 Sample : L2749-02
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4W7

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.498	43	49	56	rBV2	15539	19463	1.05%	0.117%
2	1.600	72	81	100	rBV2	318921	486948	26.15%	2.937%
3	1.700	104	112	121	rVB	50374	59723	3.21%	0.360%
4	1.932	175	184	201	rVB	128549	173059	9.29%	1.044%
5	2.591	373	389	399	rBV	256762	429842	23.09%	2.593%
6	2.652	399	408	425	rVB	160801	270835	14.55%	1.633%
7	3.208	562	581	598	rBV	317016	706537	37.95%	4.261%
8	3.616	695	708	724	rBV3	11298	25481	1.37%	0.154%
9	4.481	954	977	1009	rBV	712263	1861930	100.00%	11.230%
10	4.661	1017	1033	1051	rBV	259010	619565	33.28%	3.737%
11	4.742	1054	1058	1079	rVB2	25393	50186	2.70%	0.303%
12	5.102	1154	1170	1188	rBV	240799	515435	27.68%	3.109%
13	5.427	1253	1271	1286	rBV5	22692	52598	2.82%	0.317%
14	5.761	1352	1375	1407	rBV2	477409	1258026	67.57%	7.588%
15	6.279	1517	1536	1563	rVV	383198	786494	42.24%	4.744%
16	6.420	1567	1580	1601	rVB2	34443	69206	3.72%	0.417%
17	6.722	1659	1674	1691	rBV2	299344	584599	31.40%	3.526%
18	7.156	1790	1809	1817	rBV	697589	1437685	77.21%	8.671%
19	7.591	1931	1944	1957	rBV	165664	288290	15.48%	1.739%
20	7.922	2033	2047	2061	rBV	604689	1075896	57.78%	6.489%
21	7.989	2062	2068	2079	rVV2	37966	70558	3.79%	0.426%
22	8.201	2121	2134	2147	rBV2	107849	186341	10.01%	1.124%
23	8.443	2197	2209	2217	rBV4	12904	23376	1.26%	0.141%
24	8.497	2218	2226	2240	rVB4	16282	37614	2.02%	0.227%
25	8.655	2260	2275	2287	rBV	819439	1431453	76.88%	8.634%
26	8.806	2314	2322	2332	rVB3	24809	37137	1.99%	0.224%
27	9.436	2505	2518	2538	rBV	550175	941641	50.57%	5.679%
28	10.359	2793	2805	2821	rVB4	22834	37494	2.01%	0.226%
29	10.462	2827	2837	2850	rVB	13813	22598	1.21%	0.136%
30	10.770	2921	2933	2946	rBV	239730	384005	20.62%	2.316%
31	10.902	2959	2974	2989	rBV3	28364	48127	2.58%	0.290%
32	11.041	3003	3017	3029	rVB2	11880	22808	1.22%	0.138%
33	11.700	3208	3222	3231	rBV5	13137	20180	1.08%	0.122%
34	11.825	3248	3261	3279	rVB	613923	1023555	54.97%	6.173%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR050720WMA.M
Title : TRACE VOA SOM01.0

35	12.082	3327	3341	3356	rBV4	13188	31436	1.69%	0.190%
36	12.204	3364	3379	3396	rBV	619191	1004872	53.97%	6.061%
37	12.462	3448	3459	3469	rBV4	12503	20254	1.09%	0.122%
38	12.520	3469	3477	3487	rBV	26113	40485	2.17%	0.244%
39	12.796	3552	3563	3574	rBV3	23374	43370	2.33%	0.262%
40	12.912	3587	3599	3606	rBV3	17740	27568	1.48%	0.166%
41	14.114	3963	3973	3988	rBV	75964	122157	6.56%	0.737%
42	14.356	4037	4048	4061	rBV	132654	209575	11.26%	1.264%
43	16.751	4786	4793	4805	rBV6	11498	21802	1.17%	0.131%

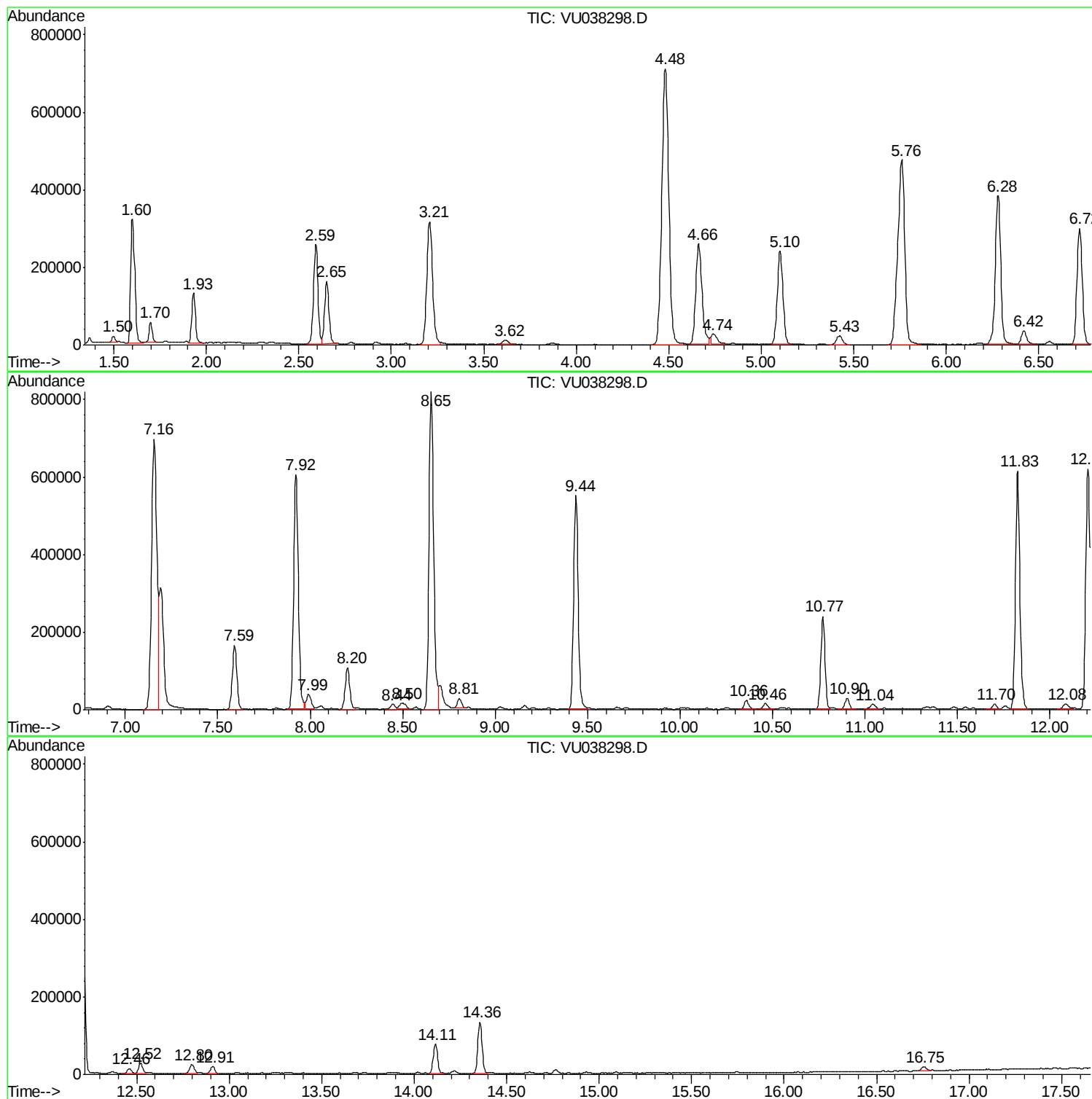
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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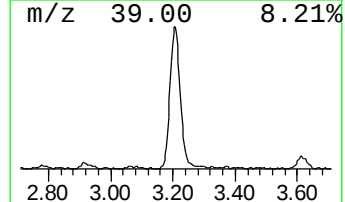
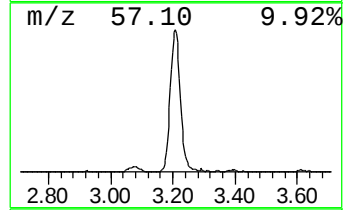
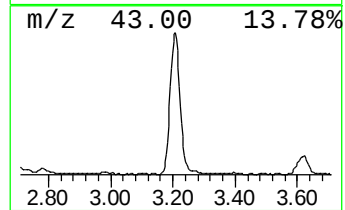
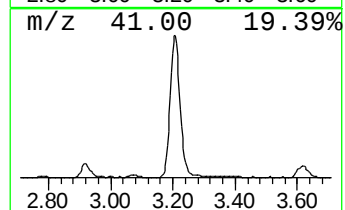
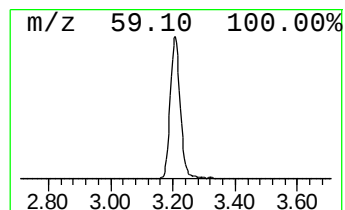
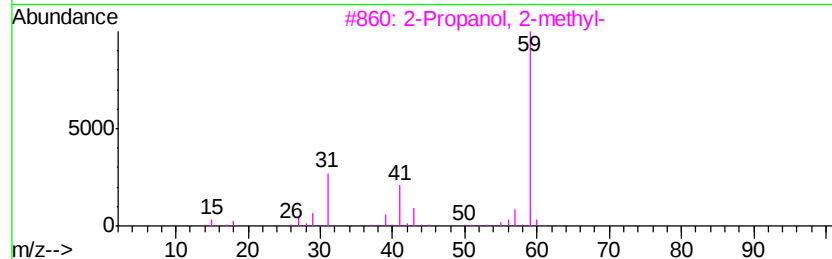
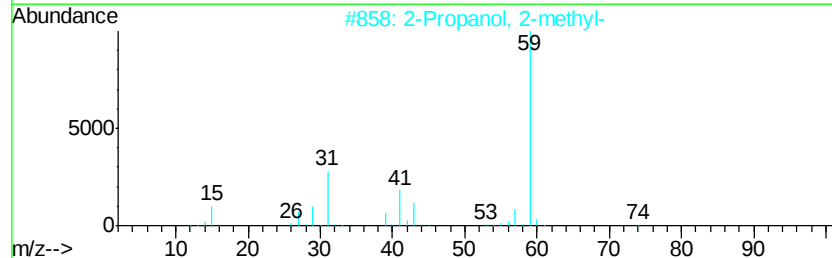
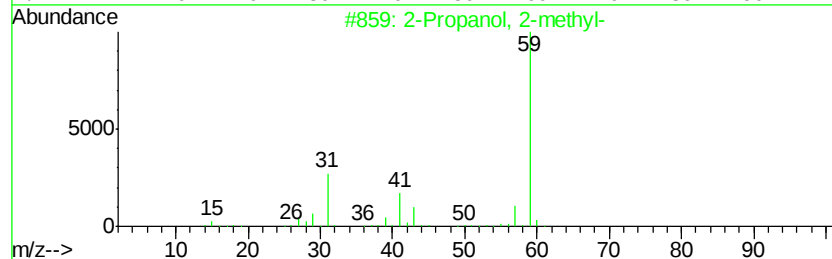
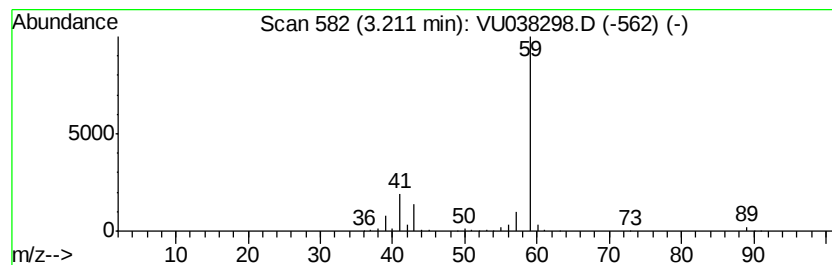
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.21	4.49 ug/L	706537	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	78
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	37
5			4-Pentene-2-ol, 2-methyl	100	C6H12O	000624-97-5	9



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Instrument :
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ClientSampleId :
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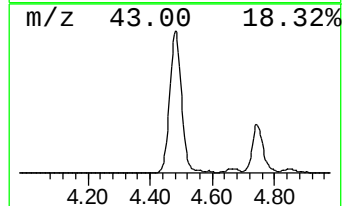
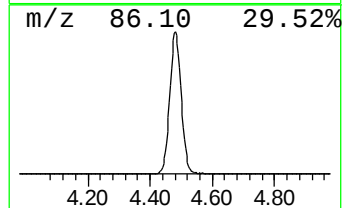
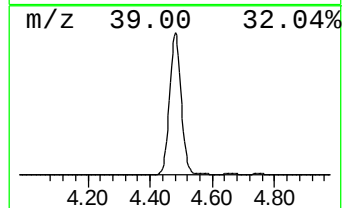
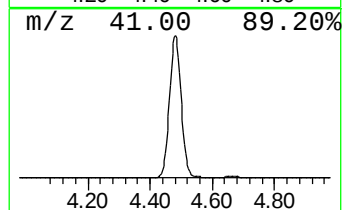
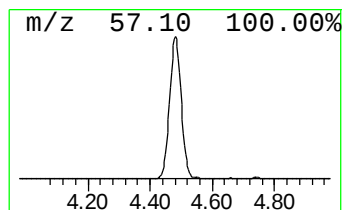
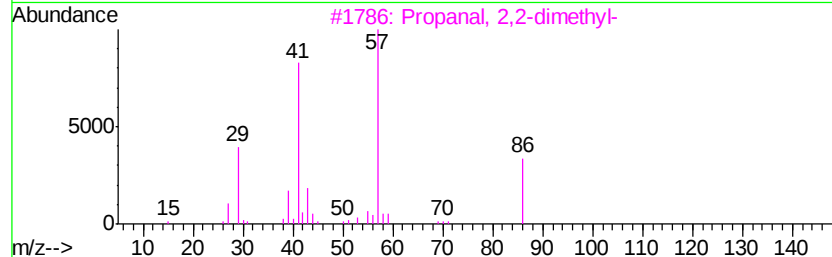
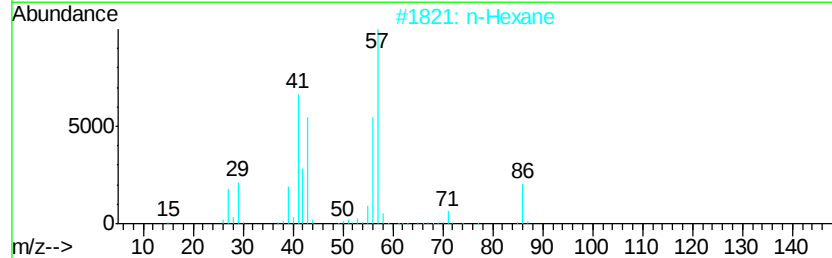
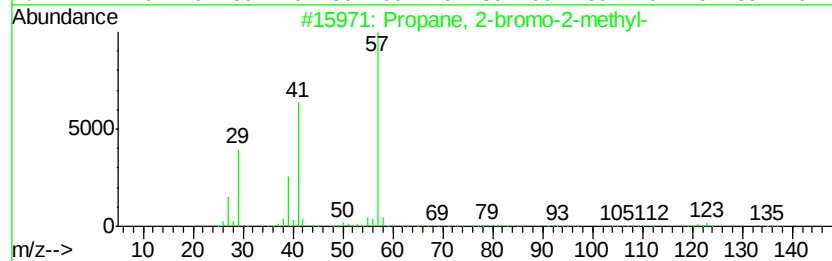
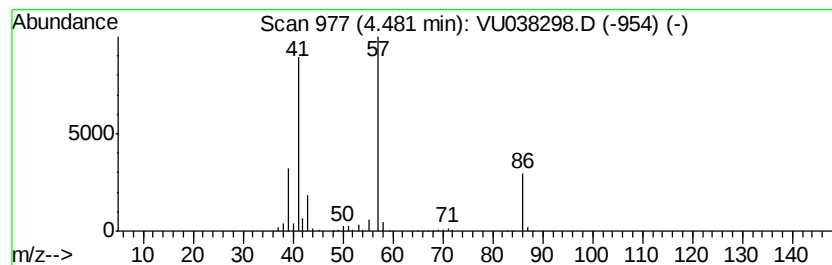
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 2-bromo-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	11.84 ug/L	1861930	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
2		n-Hexane	86	C6H14	000110-54-3	53
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
4		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	45
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	45



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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
BE4W7

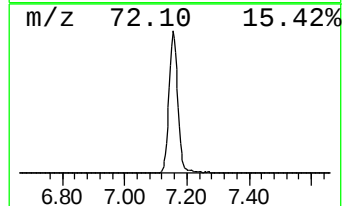
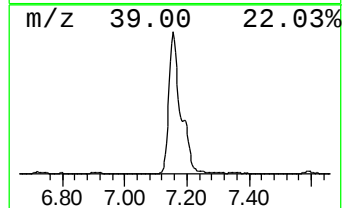
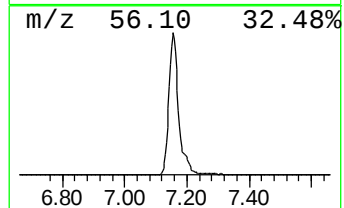
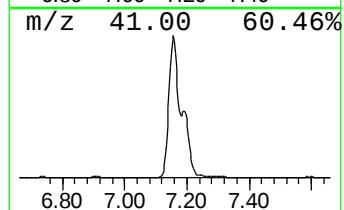
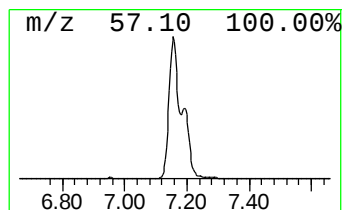
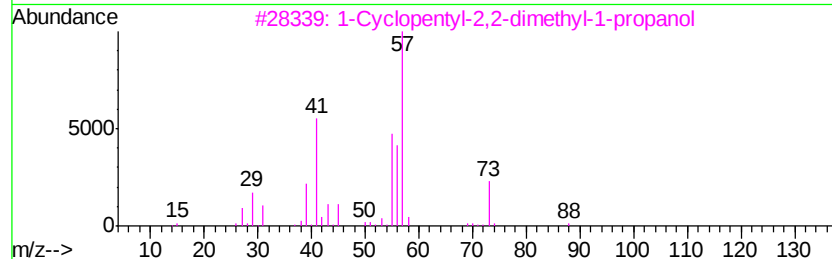
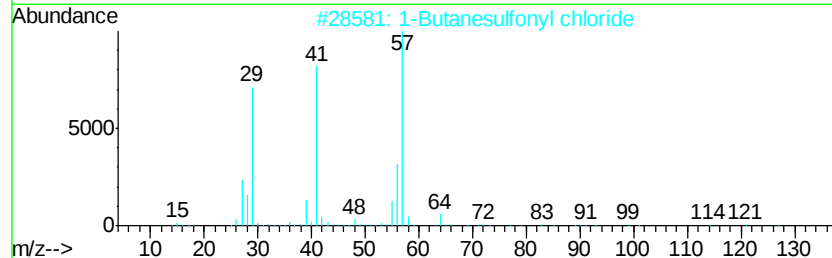
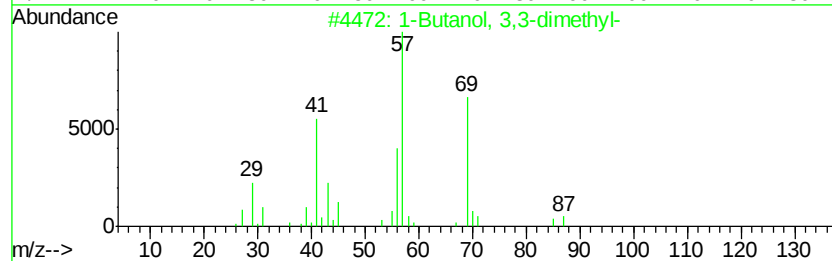
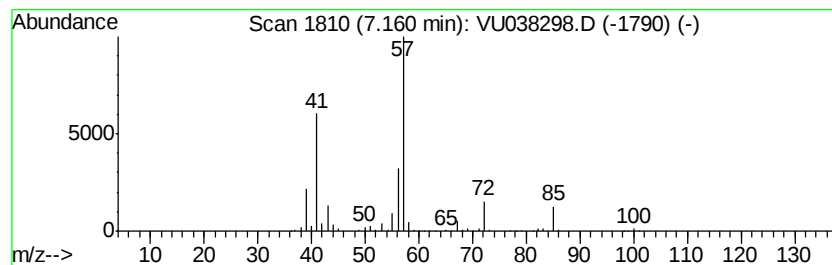
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	9.14 ug/L	1437690	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	40
2			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	38
3			1-Cyclopentyl-2,2-dimethyl-1-propanol	156	C10H20O	337966-85-5	38
4			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	38
5			Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	37



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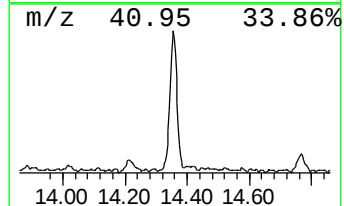
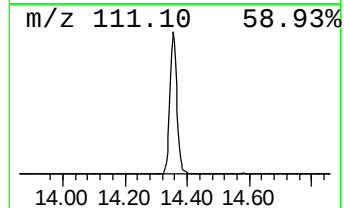
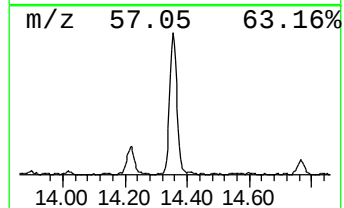
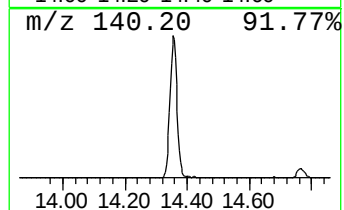
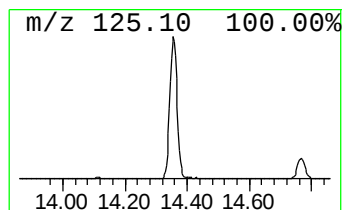
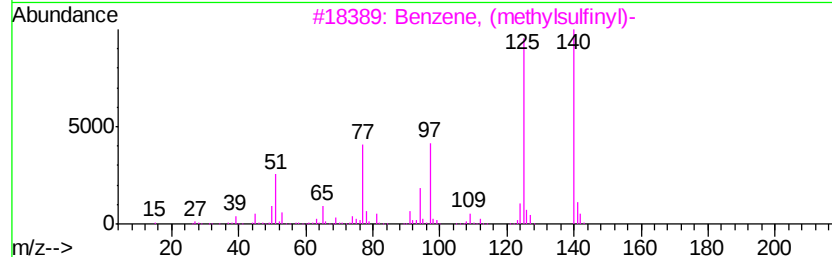
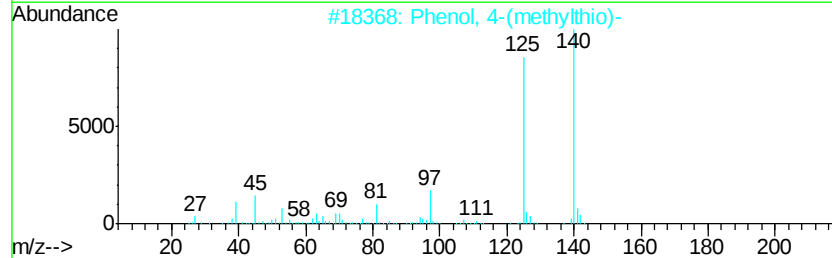
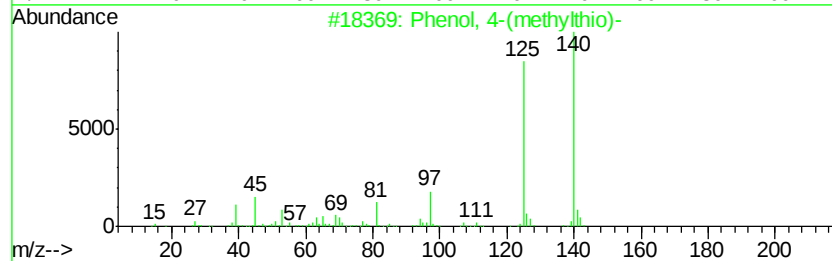
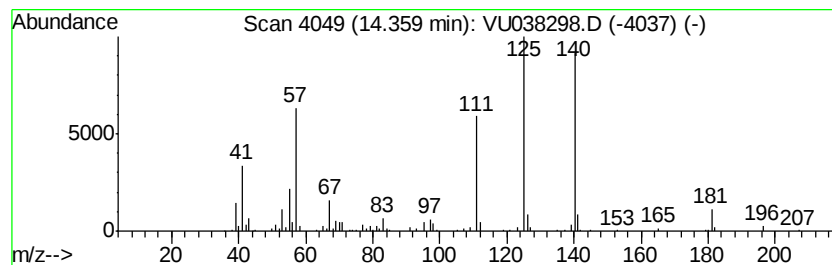
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Phenol, 4-(methylthio)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	1.02 ug/L	209575	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	64
2		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
3		Benzene, (methylsulfinyl)-	140	C7H8OS	001193-82-4	59
4		3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	59
5		Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	59



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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-met...	3.21	4.5	ug/L	706537	1	6.28	786494	5.0
Propane, 2-bromo-...	4.48	11.8	ug/L	1861930	1	6.28	786494	5.0
unknown-01	7.16	9.1	ug/L	1437690	1	6.28	786494	5.0
Phenol, 4-(methyl...	14.36	1.0	ug/L	209575	3	11.83	1023560	5.0