

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052620\
 Data File : VU038297.D
 Acq On : 26 May 2020 15:27
 Operator : JC/MD
 Sample : L2749-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4W6

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	42	49	57	rBV3	18736	25617	1.35%	0.158%
2	1.597	72	80	97	rBV2	327249	487186	25.65%	3.014%
3	1.700	104	112	123	rVB	50566	59892	3.15%	0.371%
4	1.928	175	183	196	rVB	122248	160558	8.45%	0.993%
5	2.591	371	389	399	rBV	242532	404346	21.29%	2.502%
6	2.652	399	408	429	rVB	161698	278247	14.65%	1.721%
7	3.208	562	581	612	rBV	321507	715344	37.66%	4.426%
8	3.616	696	708	727	rVB4	11628	28972	1.53%	0.179%
9	4.481	956	977	1006	rBV	726511	1899377	100.00%	11.751%
10	4.661	1017	1033	1050	rBV	249121	584059	30.75%	3.613%
11	4.742	1052	1058	1075	rVB	23287	53720	2.83%	0.332%
12	5.102	1155	1170	1191	rBV	226572	492585	25.93%	3.047%
13	5.423	1257	1270	1283	rBV3	22369	50837	2.68%	0.315%
14	5.761	1352	1375	1392	rBV2	452185	1172520	61.73%	7.254%
15	6.282	1516	1537	1564	rVB2	400491	798157	42.02%	4.938%
16	6.420	1568	1580	1594	rBV	34247	64633	3.40%	0.400%
17	6.722	1659	1674	1690	rBV	285274	555393	29.24%	3.436%
18	7.157	1791	1809	1817	rBV	705640	1413916	74.44%	8.747%
19	7.594	1931	1945	1962	rBV	154534	269950	14.21%	1.670%
20	7.925	2033	2048	2062	rBV	574765	1011577	53.26%	6.258%
21	7.993	2062	2069	2080	rVV	38600	72953	3.84%	0.451%
22	8.205	2120	2135	2146	rBV	100579	174781	9.20%	1.081%
23	8.449	2199	2211	2217	rBV2	11009	19020	1.00%	0.118%
24	8.655	2261	2275	2288	rBV	791645	1372470	72.26%	8.491%
25	8.809	2314	2323	2332	rVB4	26343	39524	2.08%	0.245%
26	9.439	2505	2519	2551	rVB	561695	960319	50.56%	5.941%
27	10.362	2793	2806	2819	rBV3	23752	39956	2.10%	0.247%
28	10.465	2830	2838	2854	rVB2	12897	21012	1.11%	0.130%
29	10.774	2922	2934	2946	rBV	224249	361920	19.05%	2.239%
30	10.906	2963	2975	2986	rBV2	32354	53423	2.81%	0.331%
31	11.044	3006	3018	3028	rVB2	11558	20519	1.08%	0.127%
32	11.700	3208	3222	3232	rBV9	12597	21913	1.15%	0.136%
33	11.825	3249	3261	3281	rVB	615400	1039687	54.74%	6.432%
34	12.086	3326	3342	3363	rBV3	12567	31265	1.65%	0.193%

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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	12.208	3367	3380	3395	rBV	580295	948629	49.94%	5.869%
36	12.462	3449	3459	3469	rBV3	13174	21422	1.13%	0.133%
37	12.526	3469	3479	3491	rBV	25513	42056	2.21%	0.260%
38	12.806	3554	3566	3580	rBV2	25131	48058	2.53%	0.297%
39	12.915	3592	3600	3613	rVB6	18387	28616	1.51%	0.177%
40	14.124	3964	3976	3988	rBV	74681	120976	6.37%	0.748%
41	14.365	4038	4051	4067	rBV	123006	198298	10.44%	1.227%

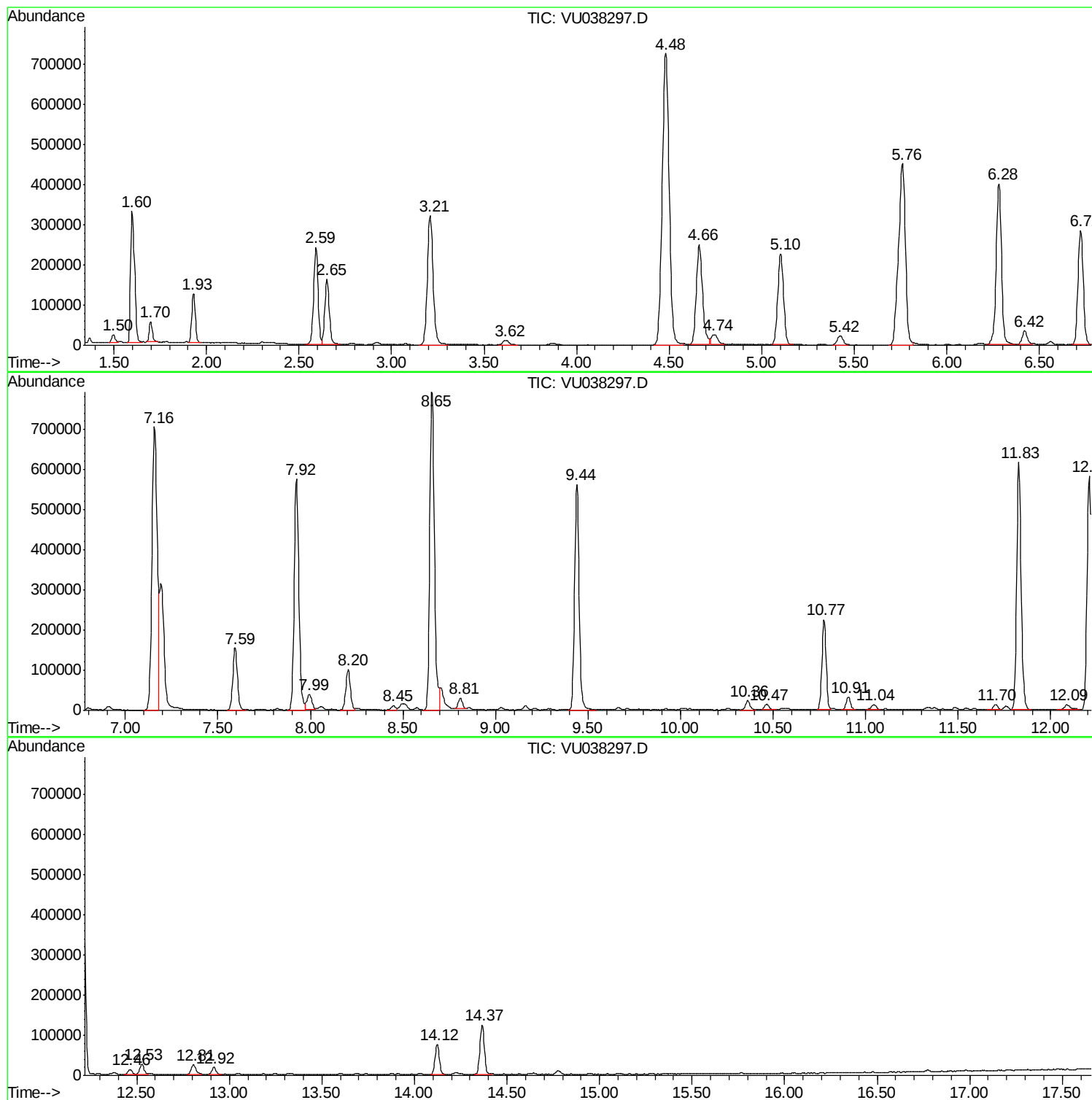
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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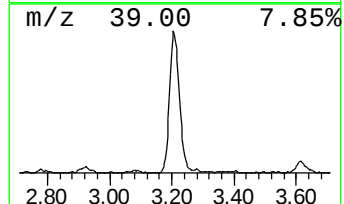
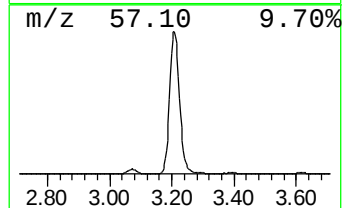
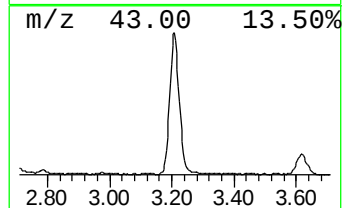
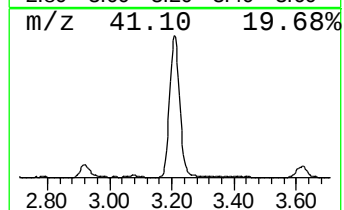
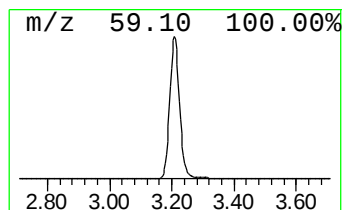
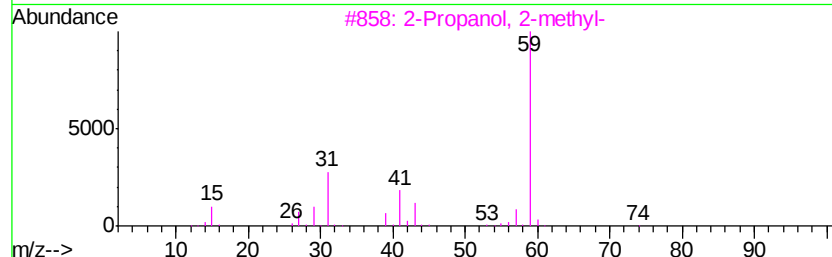
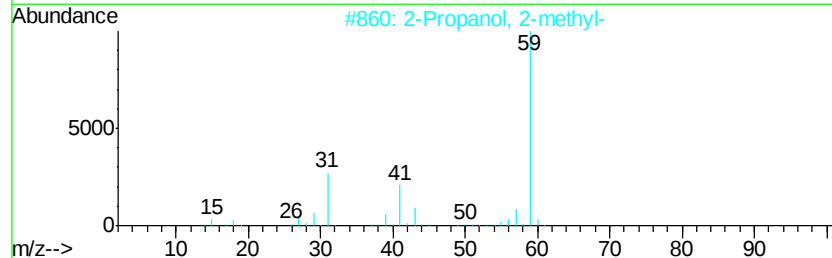
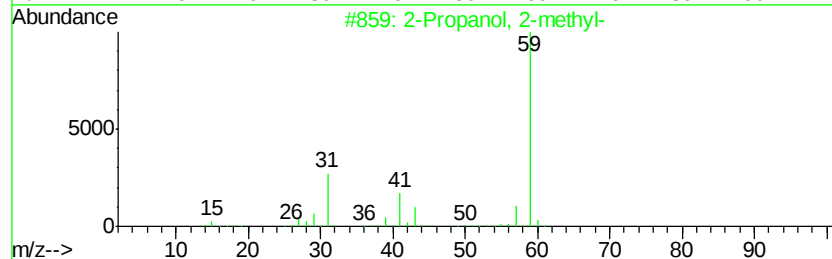
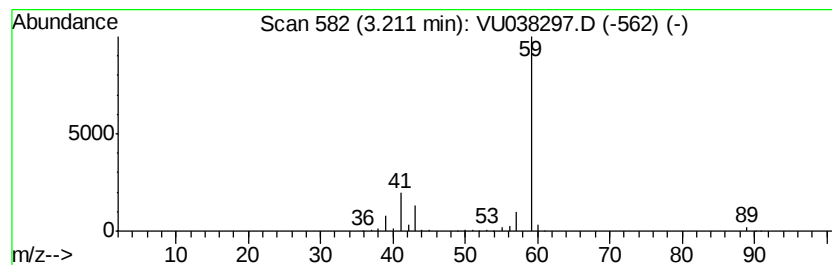
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	4.48 ug/L	715344	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
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	43
5			3-Pentanol	88	C5H12O	000584-02-1	9



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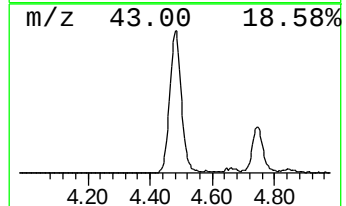
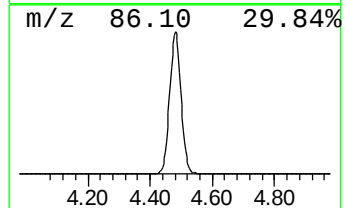
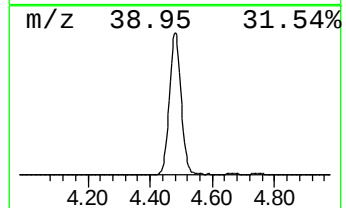
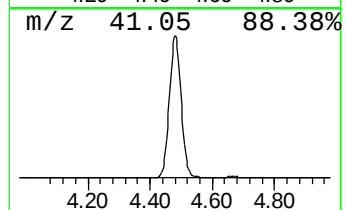
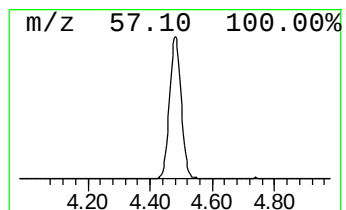
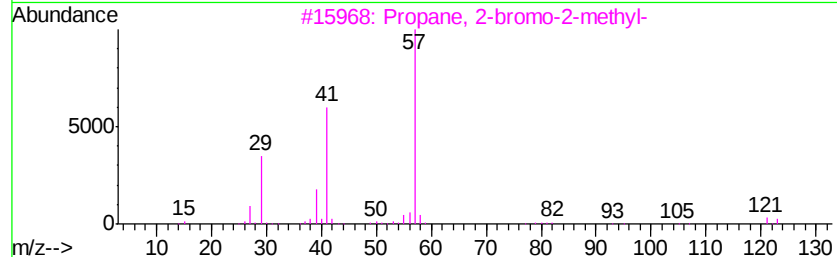
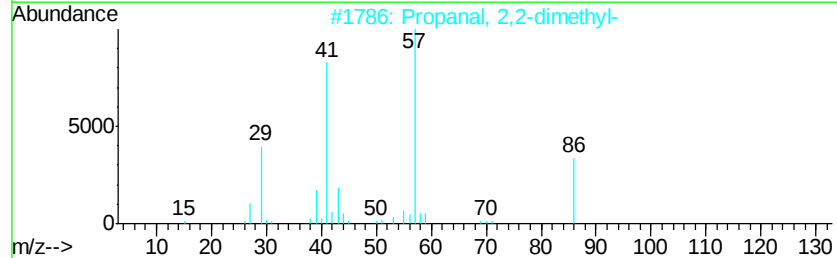
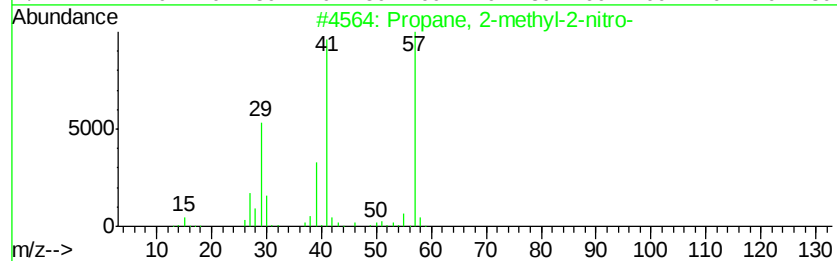
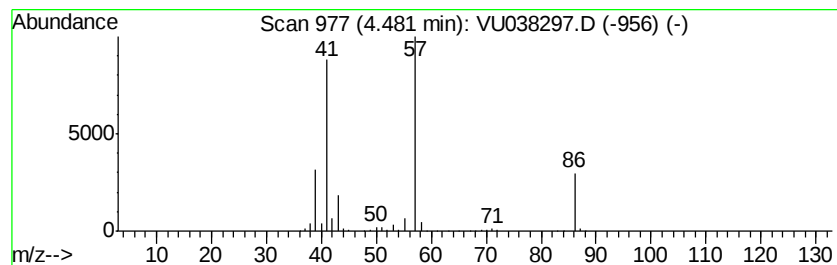
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	11.90 ug/L	1899380	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	59
2		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
3		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	42
4		3-Pentanone	86	C5H10O	000096-22-0	40
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40



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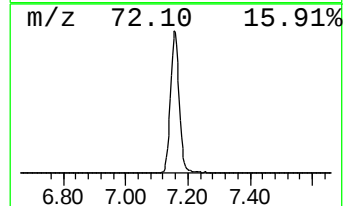
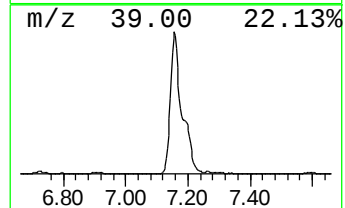
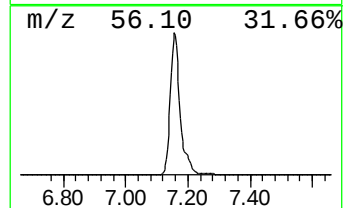
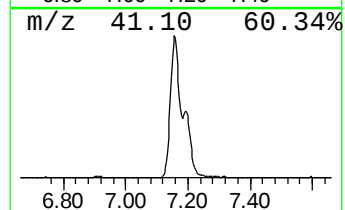
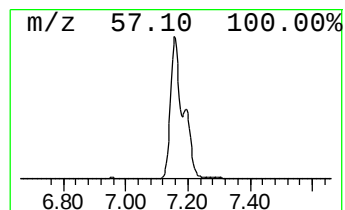
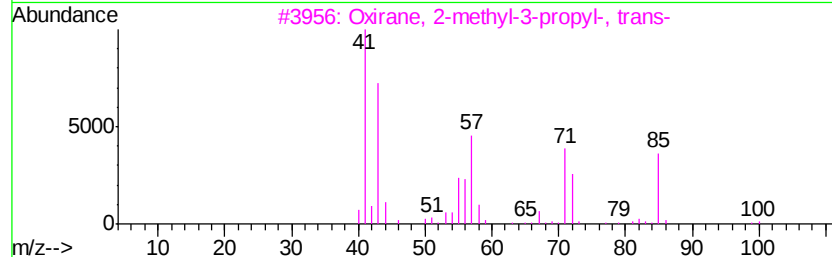
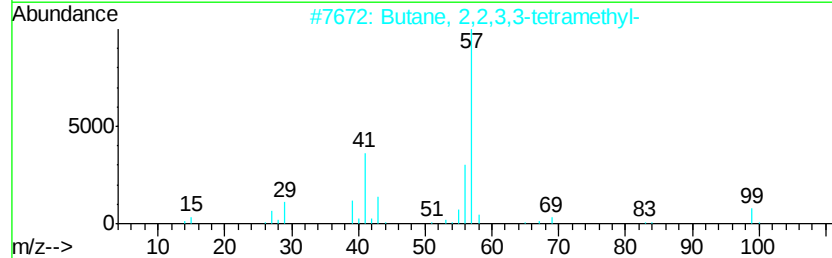
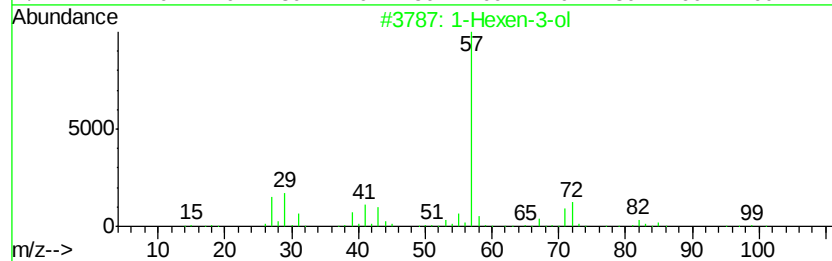
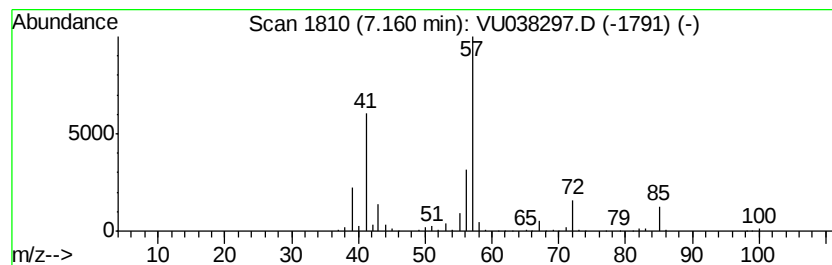
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	8.86 ug/L	1413920	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexen-3-ol	100	C6H12O	004798-44-1	37
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	37
3		Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	37
4		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	37
5		1-Hexen-3-ol	100	C6H12O	004798-44-1	37



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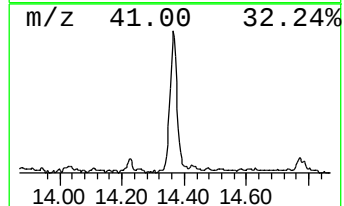
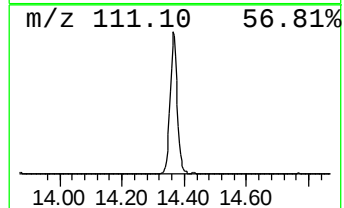
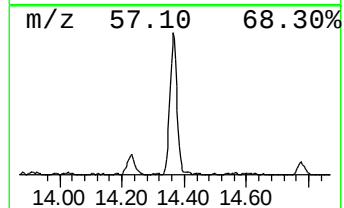
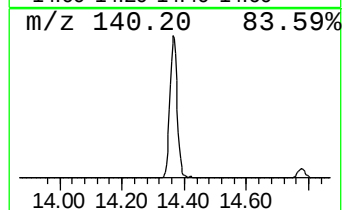
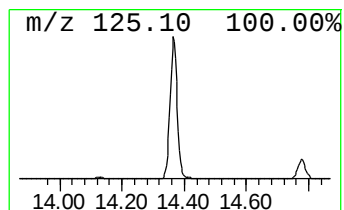
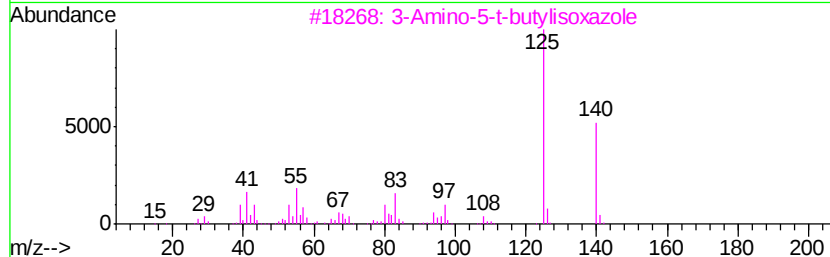
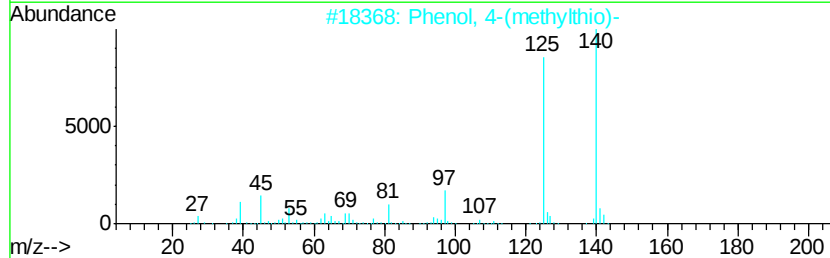
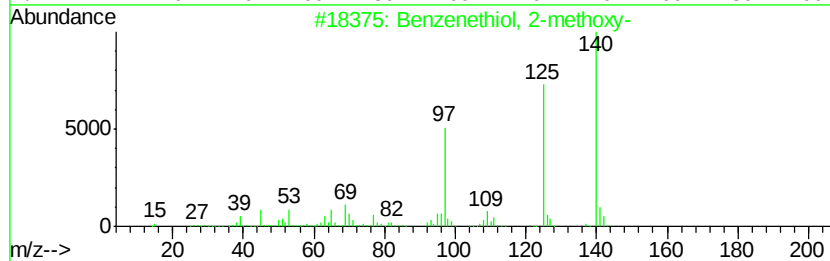
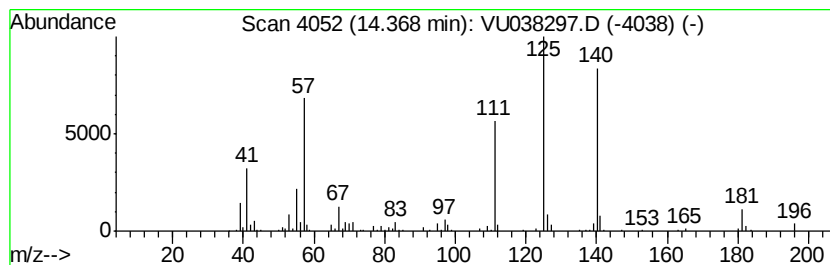
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenethiol, 2-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	0.95 ug/L	198298	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	59
2		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	53
3		3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	53
4		Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	53
5		Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	43



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
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	715344	1	6.28	798157	5.0
Propane, 2-methyl...	4.48	11.9	ug/L	1899380	1	6.28	798157	5.0
unknown-01	7.16	8.9	ug/L	1413920	1	6.28	798157	5.0
Benzenethiol, 2-m...	14.37	0.9	ug/L	198298	3	11.83	1039690	5.0