

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052720\
 Data File : VU038315.D
 Acq On : 27 May 2020 13:04
 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	1.501	43	50	56	rBV2	15060	20516	1.11%	0.128%
2	1.598	72	80	100	rBV2	266808	421763	22.83%	2.633%
3	1.700	104	112	124	rVV	51039	62129	3.36%	0.388%
4	1.932	175	184	197	rVB	117770	157884	8.55%	0.986%
5	2.591	373	389	399	rBV	237226	393976	21.33%	2.460%
6	2.649	399	407	423	rVB	160911	270667	14.65%	1.690%
7	3.205	564	580	610	rBV	317549	715449	38.73%	4.467%
8	3.617	695	708	731	rVB3	11664	27282	1.48%	0.170%
9	4.482	955	977	1004	rBV	706652	1847076	100.00%	11.533%
10	4.662	1017	1033	1050	rBV	250933	598277	32.39%	3.735%
11	4.742	1052	1058	1080	rVB	25184	55378	3.00%	0.346%
12	5.102	1153	1170	1189	rBV	229776	498113	26.97%	3.110%
13	5.424	1253	1270	1287	rBV4	22691	51124	2.77%	0.319%
14	5.761	1352	1375	1409	rBV2	450780	1188145	64.33%	7.418%
15	6.282	1515	1537	1563	rVV	367200	741140	40.13%	4.627%
16	6.417	1568	1579	1595	rBV2	33739	65939	3.57%	0.412%
17	6.723	1659	1674	1692	rBV	288268	560789	30.36%	3.501%
18	7.157	1792	1809	1817	rBV	679578	1425764	77.19%	8.902%
19	7.591	1931	1944	1958	rBV	153640	267221	14.47%	1.668%
20	7.922	2033	2047	2061	rBV	566422	1018982	55.17%	6.362%
21	7.990	2062	2068	2081	rVV	36634	68019	3.68%	0.425%
22	8.202	2120	2134	2145	rBV	101059	175404	9.50%	1.095%
23	8.446	2198	2210	2218	rBV5	10086	19532	1.06%	0.122%
24	8.504	2218	2228	2241	rVB6	11993	27427	1.48%	0.171%
25	8.652	2261	2274	2287	rBV	817830	1420766	76.92%	8.871%
26	8.806	2313	2322	2331	rVV3	25967	40096	2.17%	0.250%
27	9.436	2504	2518	2550	rVB	532357	908718	49.20%	5.674%
28	10.359	2793	2805	2820	rVB3	22073	36184	1.96%	0.226%
29	10.459	2827	2836	2848	rBV	12965	22058	1.19%	0.138%
30	10.771	2921	2933	2945	rBV	233431	379049	20.52%	2.367%
31	10.903	2961	2974	2986	rBV3	16248	27669	1.50%	0.173%
32	11.041	3008	3017	3029	rVB4	12380	23978	1.30%	0.150%
33	11.700	3208	3222	3232	rBV5	12641	21622	1.17%	0.135%
34	11.822	3248	3260	3280	rVB	573764	972785	52.67%	6.074%

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ALS Vial : 1 Sample Multiplier: 1

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ClientSampleId :
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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	12.079	3321	3340	3362	rBV3	13859	34909	1.89%	0.218%
36	12.205	3366	3379	3392	rBV	590255	964725	52.23%	6.023%
37	12.462	3447	3459	3467	rBV5	12387	20339	1.10%	0.127%
38	12.520	3468	3477	3488	rBV	25209	41389	2.24%	0.258%
39	12.800	3555	3564	3572	rBV2	14814	24753	1.34%	0.155%
40	12.909	3590	3598	3609	rVB5	19362	29861	1.62%	0.186%
41	14.115	3962	3973	3984	rBV2	77593	128164	6.94%	0.800%
42	14.356	4036	4048	4066	rBV	135954	217839	11.79%	1.360%
43	16.754	4786	4794	4804	rBV7	15197	23307	1.26%	0.146%

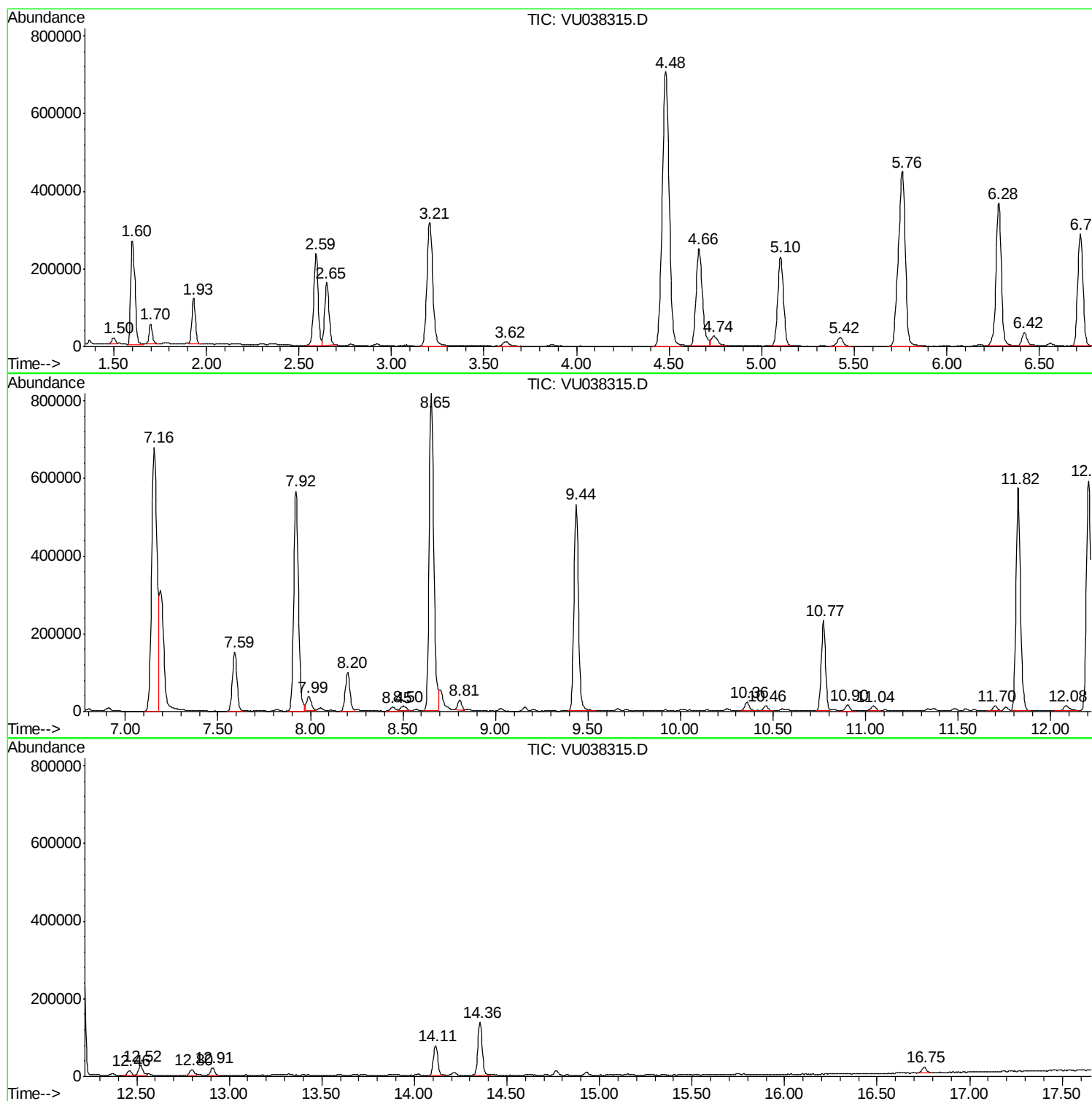
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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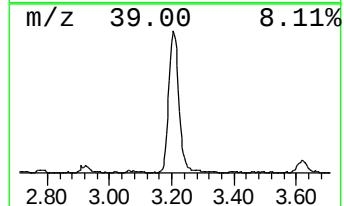
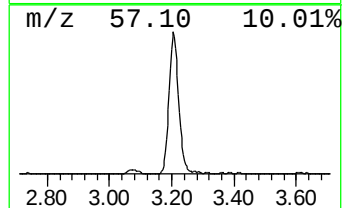
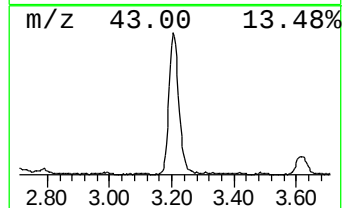
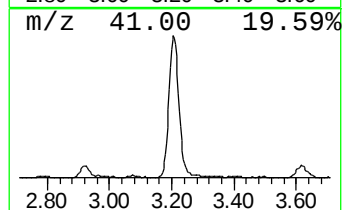
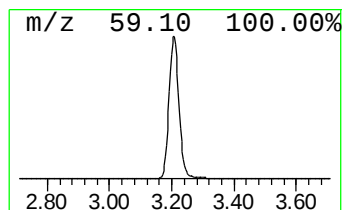
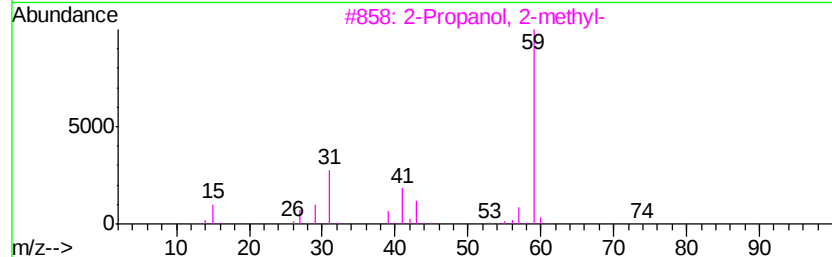
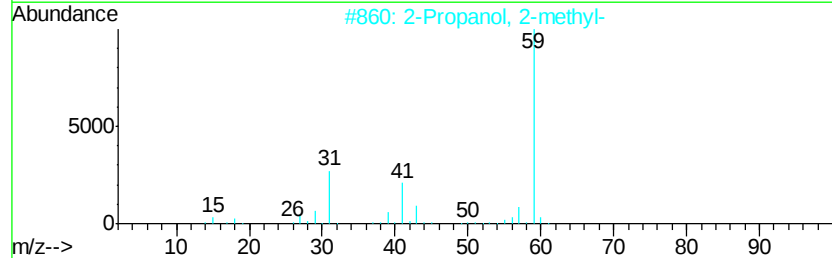
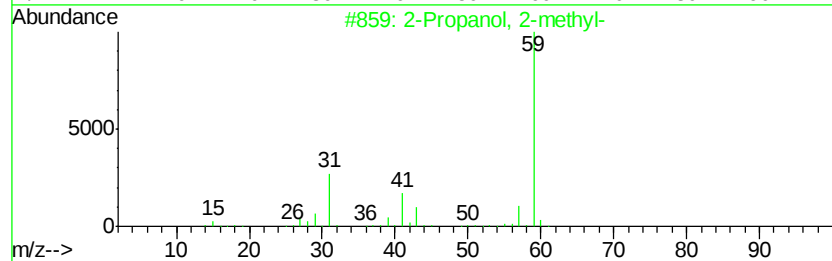
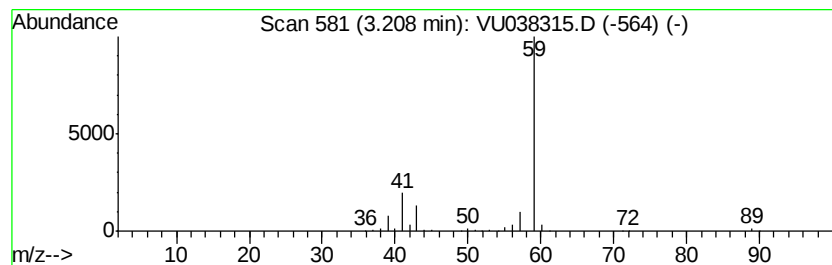
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	4.83 ug/L	715449	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	83
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	74
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	37
5			3-Pentanol	88	C5H12O	000584-02-1	9



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Instrument :
MSVOA_U
ClientSampleId :
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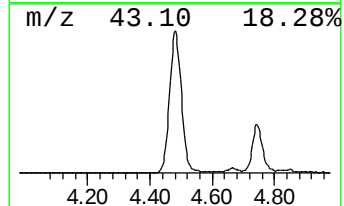
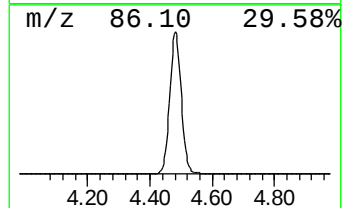
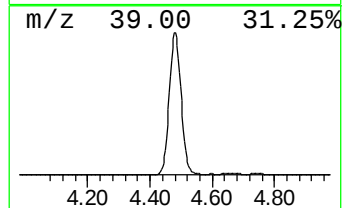
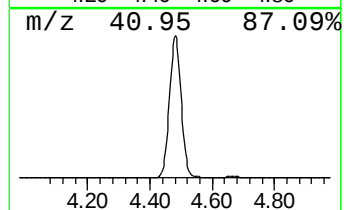
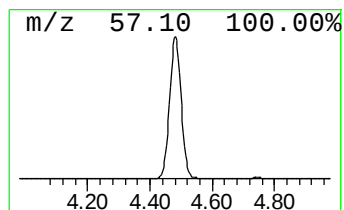
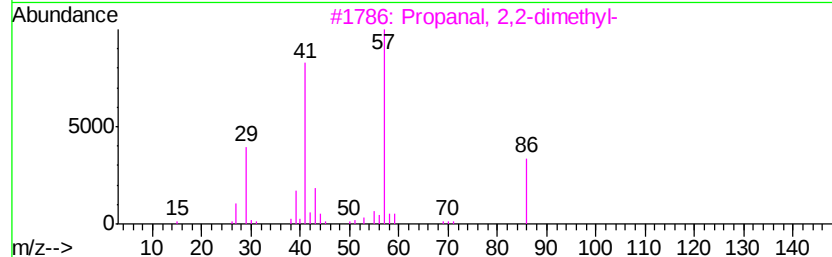
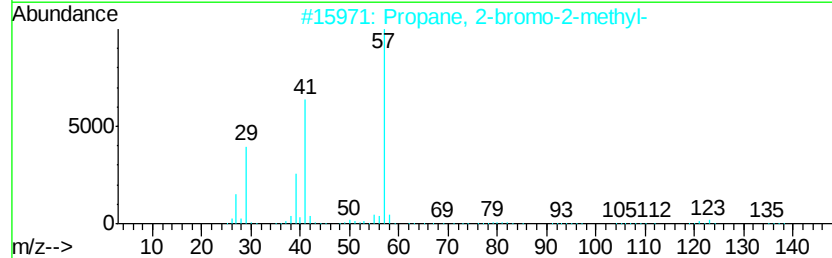
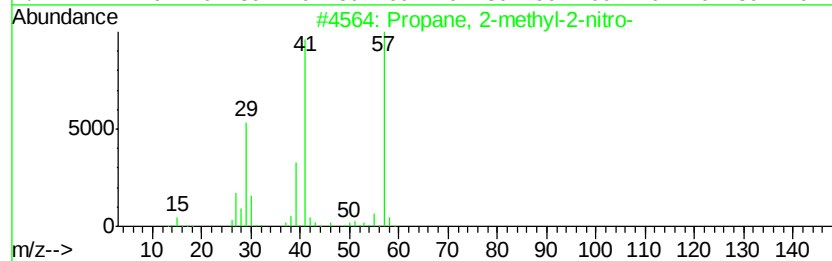
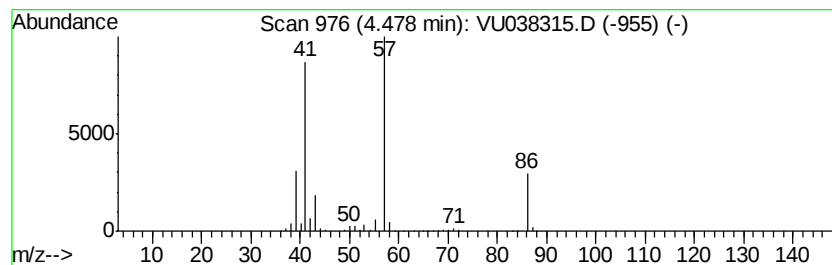
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Quant Title : TRACE VOA SOM01.0

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	12.46 ug/L	1847080	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		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
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	40



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Sample : L2749-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

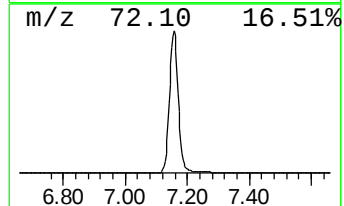
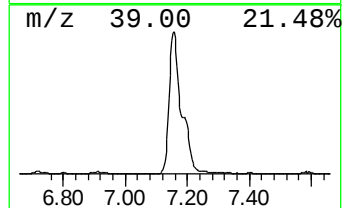
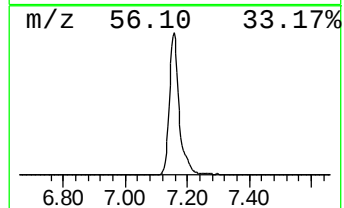
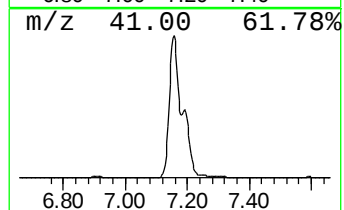
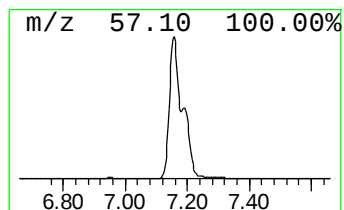
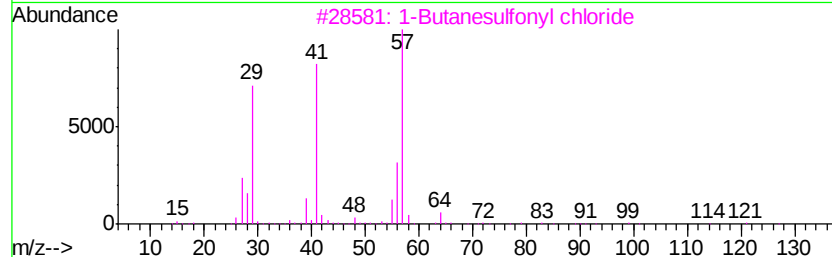
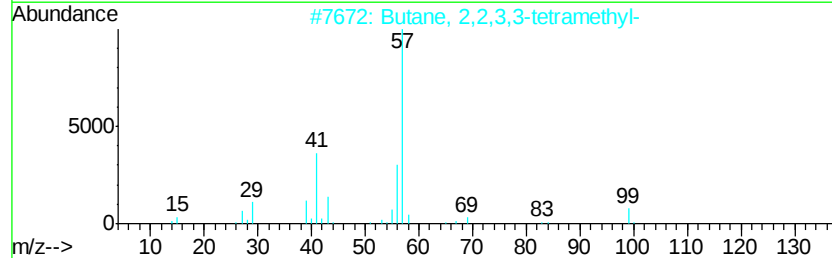
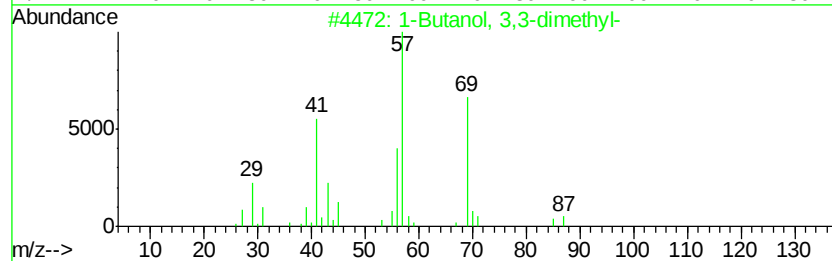
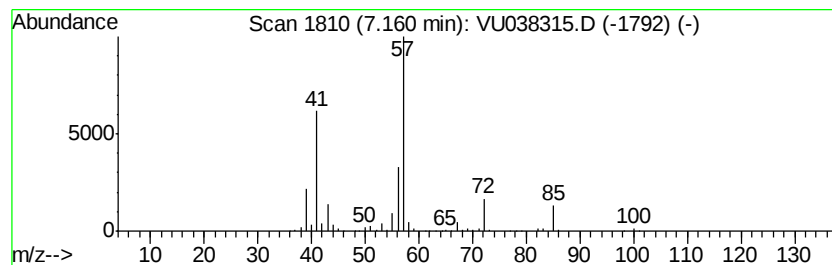
Instrument :
MSVOA_U
ClientSampled :
BE4W7

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	9.62 ug/L	1425760	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	42
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
3	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	42
4	1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	42
5	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	37



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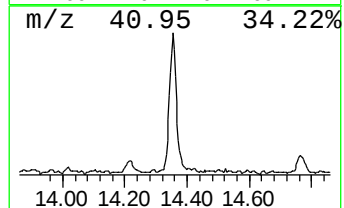
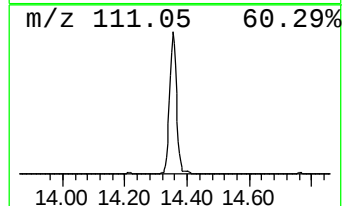
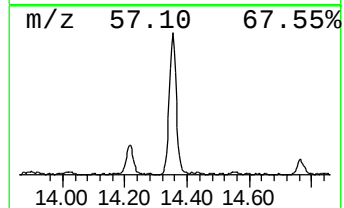
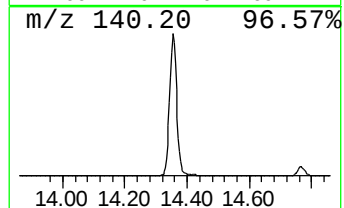
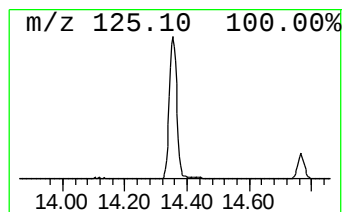
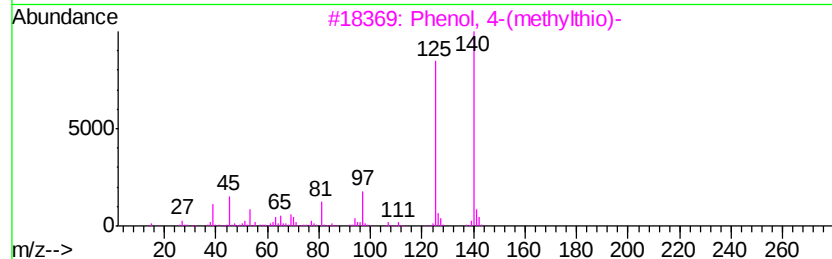
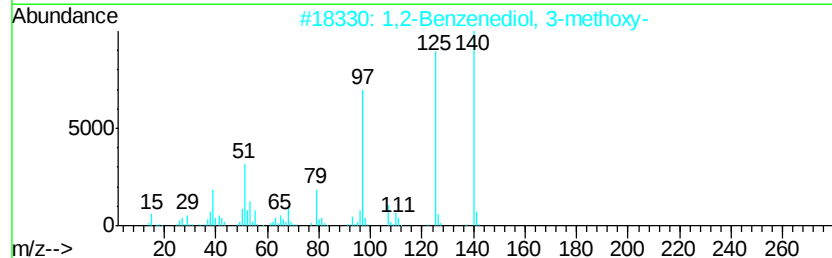
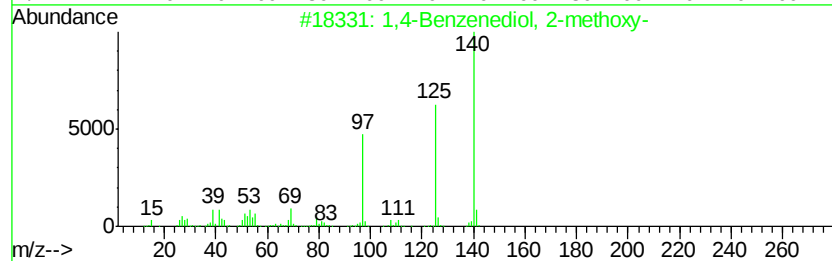
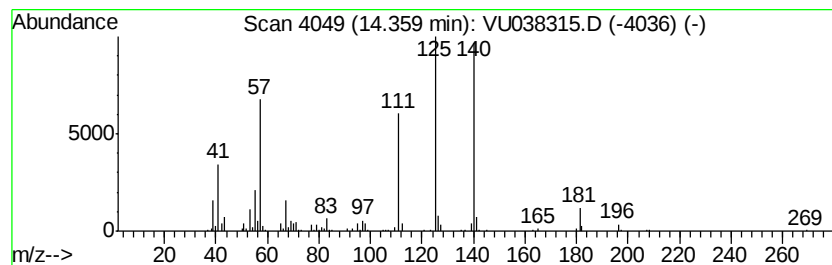
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 1,4-Benzenediol, 2-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	1.12 ug/L	217839	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	59
2		1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
3		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
4		Uracil, 5-ethyl-	140	C6H8N2O2	004212-49-1	53
5		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	45



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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	4.8	ug/L	715449	1	6.28	741140	5.0
Propane, 2-methyl...	4.48	12.5	ug/L	1847080	1	6.28	741140	5.0
unknown-01	7.16	9.6	ug/L	1425760	1	6.28	741140	5.0
1,4-Benzenediol, ...	14.36	1.1	ug/L	217839	3	11.83	972785	5.0