

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052720\
 Data File : VU038312.D
 Acq On : 27 May 2020 11:55
 Operator : JC/MD
 Sample : L2766-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4Y5

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	41	50	71	rBV4	37035	66932	3.50%	0.411%
2	1.597	72	80	99	rVV2	280701	434733	22.73%	2.672%
3	1.700	104	112	132	rVB	59080	80190	4.19%	0.493%
4	1.932	176	184	195	rVB	117355	150599	7.87%	0.926%
5	2.591	374	389	399	rBV	231232	390096	20.40%	2.398%
6	2.655	399	409	429	rVB	186889	330627	17.29%	2.033%
7	3.221	565	585	614	rBV2	309005	788055	41.20%	4.845%
8	3.616	693	708	726	rBV3	12930	30864	1.61%	0.190%
9	4.481	952	977	1003	rBV	736819	1912597	100.00%	11.758%
10	4.665	1018	1034	1051	rBV	248762	597843	31.26%	3.675%
11	5.102	1154	1170	1188	rBV	222739	490890	25.67%	3.018%
12	5.420	1252	1269	1287	rBV3	13705	31414	1.64%	0.193%
13	5.761	1352	1375	1396	rBV2	441667	1162101	60.76%	7.144%
14	6.282	1516	1537	1561	rVV	407860	816378	42.68%	5.019%
15	6.420	1569	1580	1602	rBV2	34833	70056	3.66%	0.431%
16	6.722	1658	1674	1691	rBV	279084	547658	28.63%	3.367%
17	7.160	1793	1810	1817	rBV	675144	1368398	71.55%	8.412%
18	7.594	1928	1945	1961	rBV	151210	263470	13.78%	1.620%
19	7.925	2034	2048	2062	rBV	546150	988921	51.71%	6.079%
20	7.996	2063	2070	2080	rVV	36062	66265	3.46%	0.407%
21	8.205	2122	2135	2148	rBV	97809	171663	8.98%	1.055%
22	8.449	2201	2211	2217	rBV4	13477	22737	1.19%	0.140%
23	8.497	2218	2226	2242	rVB4	20662	45192	2.36%	0.278%
24	8.658	2262	2276	2288	rBV	829107	1417820	74.13%	8.716%
25	8.809	2313	2323	2333	rBV2	27662	43432	2.27%	0.267%
26	9.439	2506	2519	2549	rBV	571415	971174	50.78%	5.970%
27	10.362	2796	2806	2818	rBV3	26316	42056	2.20%	0.259%
28	10.465	2829	2838	2847	rBV3	11878	19749	1.03%	0.121%
29	10.774	2921	2934	2946	rBV	228199	369306	19.31%	2.270%
30	10.909	2963	2976	2987	rVB3	37253	61302	3.21%	0.377%
31	11.044	3011	3018	3030	rVB3	12271	21253	1.11%	0.131%
32	11.703	3208	3223	3233	rBV6	15432	24676	1.29%	0.152%
33	11.828	3249	3262	3282	rVB	639450	1057383	55.29%	6.500%
34	12.089	3328	3343	3356	rBV3	13327	28792	1.51%	0.177%

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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	3363	3380	3393	rBV	592081	934721	48.87%	5.746%
36	12.526	3470	3479	3488	rBV	24267	37622	1.97%	0.231%
37	12.806	3556	3566	3576	rBV3	28352	46961	2.46%	0.289%
38	12.918	3592	3601	3611	rVB3	17660	28515	1.49%	0.175%
39	14.124	3964	3976	3987	rBV	83344	134235	7.02%	0.825%
40	14.365	4039	4051	4064	rBV2	123877	200295	10.47%	1.231%

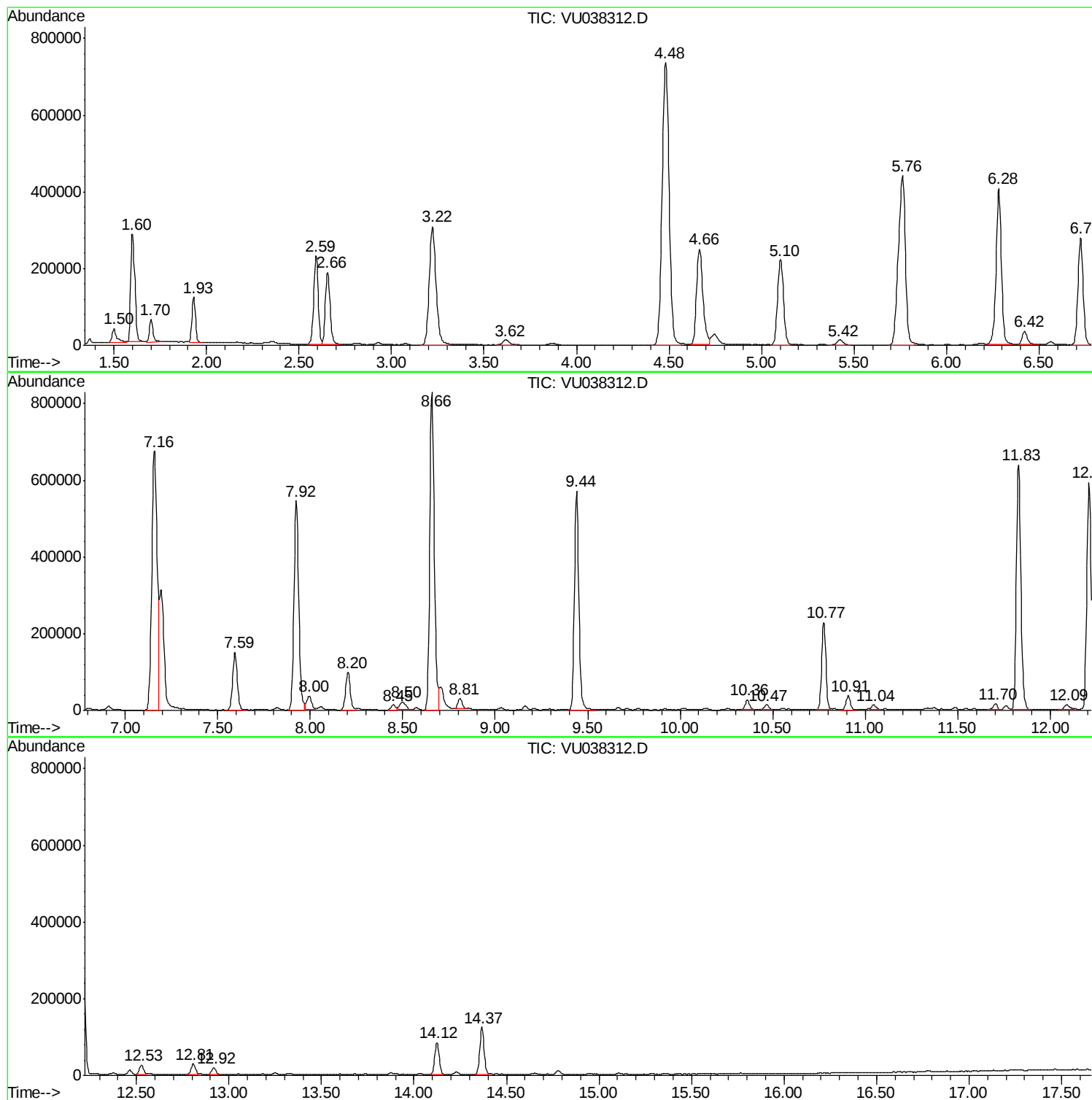
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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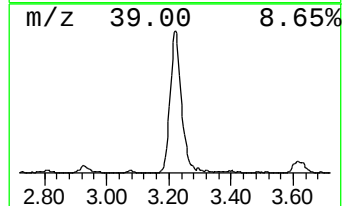
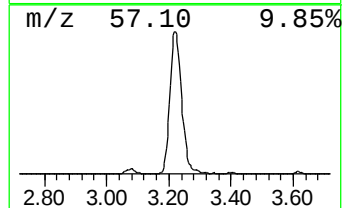
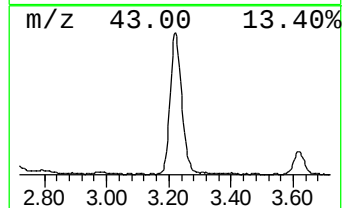
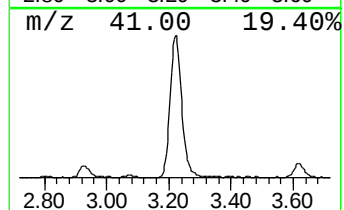
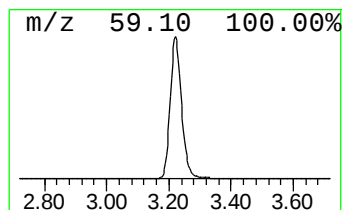
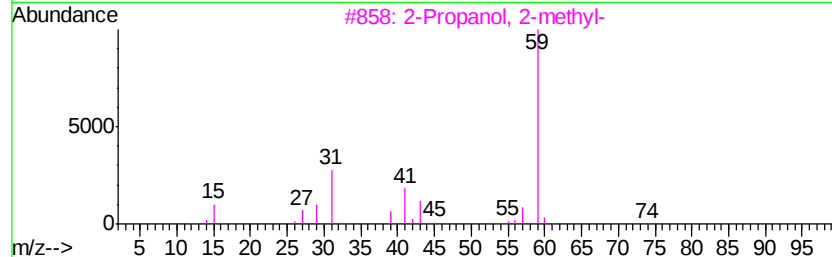
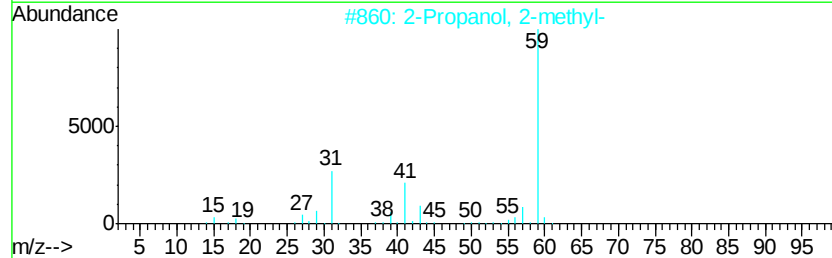
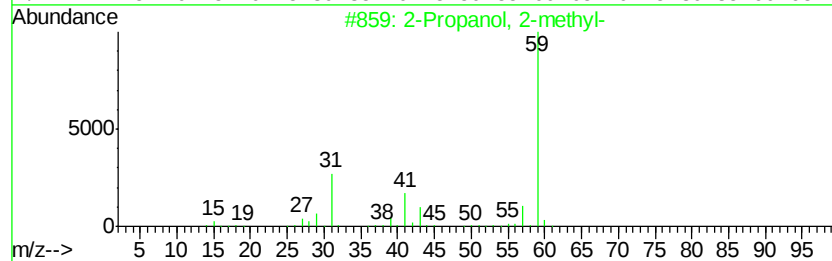
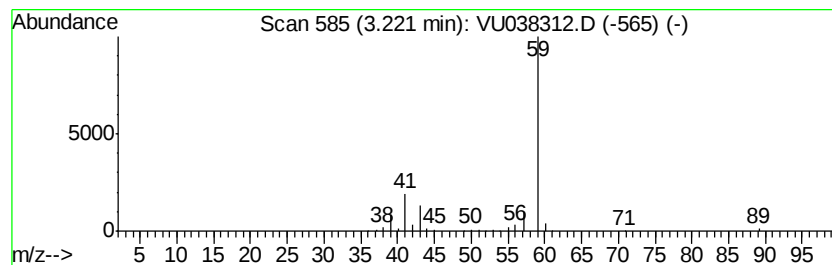
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.22	4.83 ug/L	788055	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	47
5			3-Pentanol	88	C5H12O	000584-02-1	9



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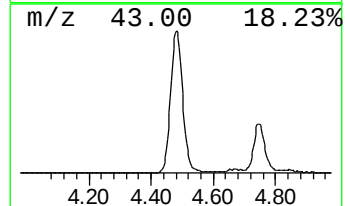
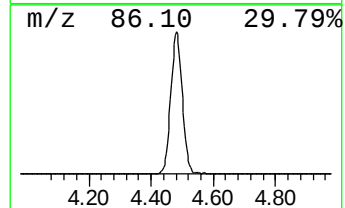
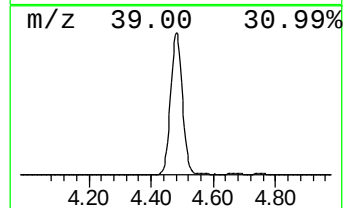
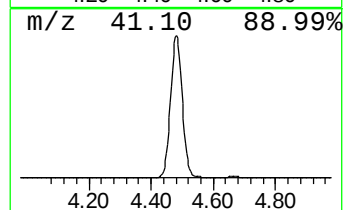
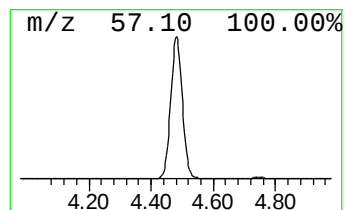
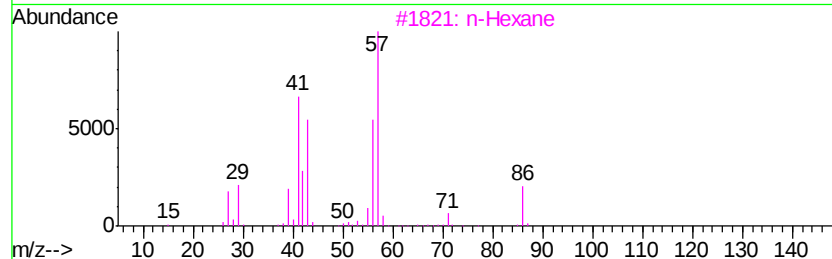
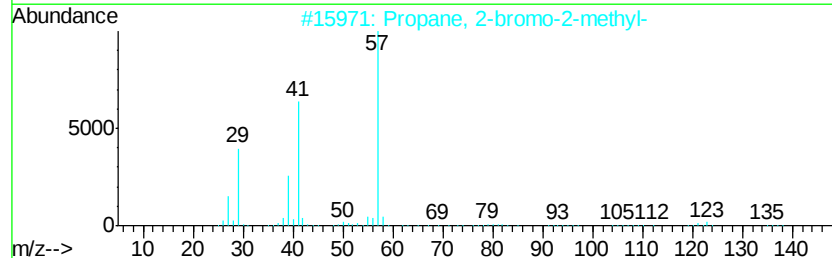
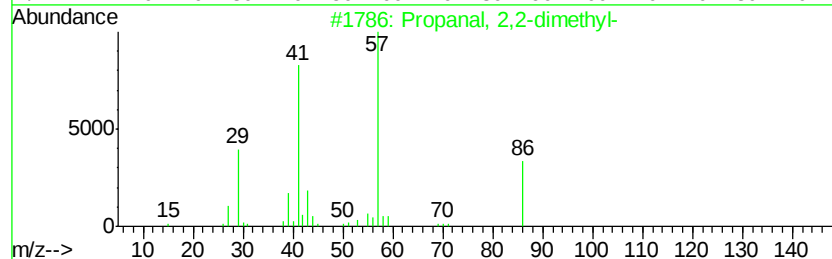
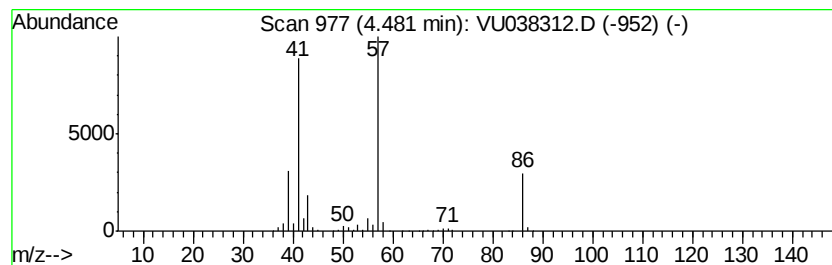
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	11.71 ug/L	1912600	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
3		n-Hexane	86	C6H14	000110-54-3	53
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	45



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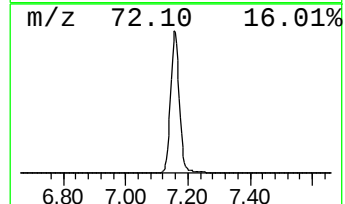
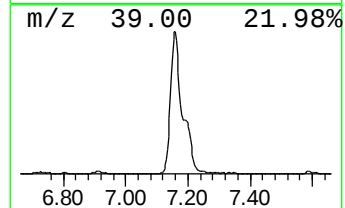
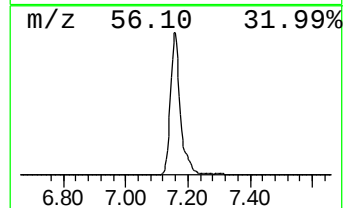
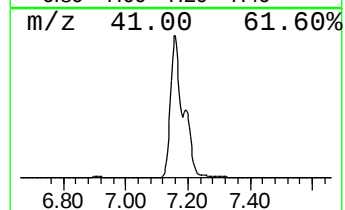
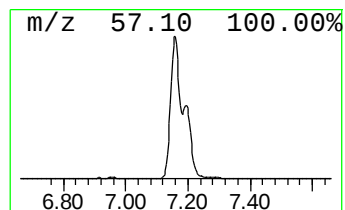
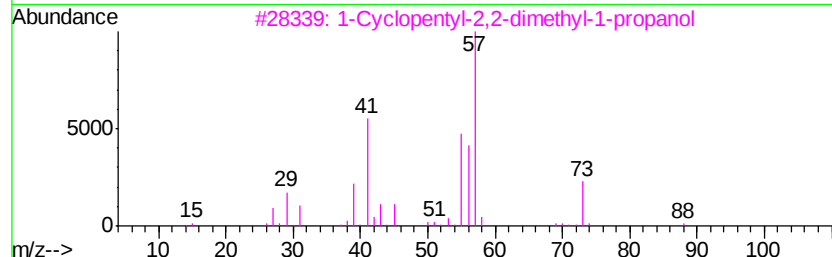
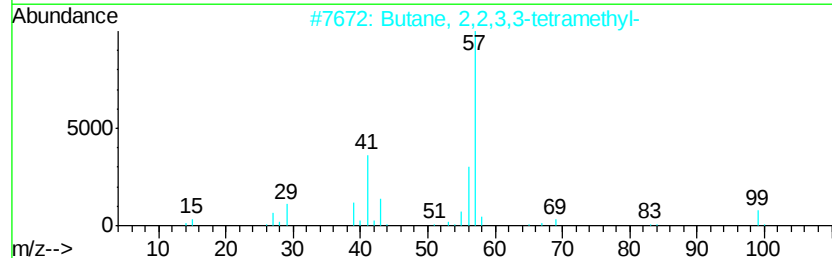
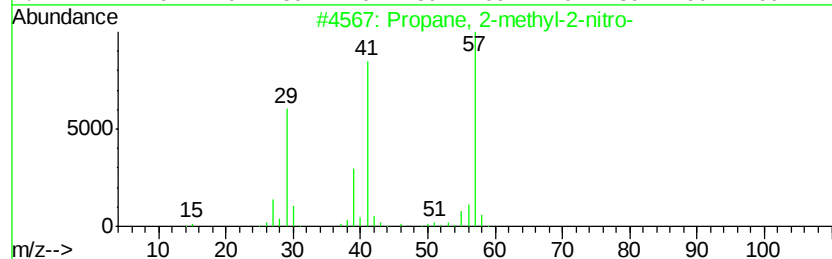
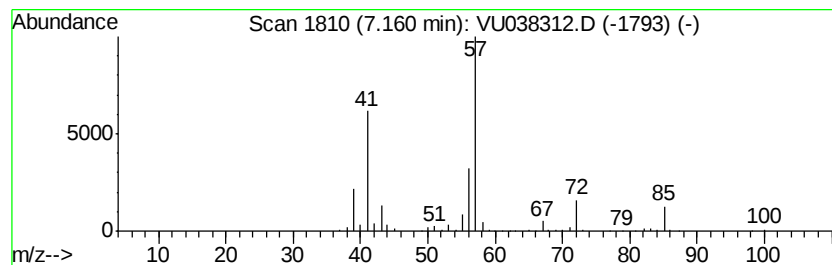
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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	8.38 ug/L	1368400	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	43
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
3		1-Cyclopentyl-2,2-dimethyl-1-propanol	156	C10H20O	337966-85-5	40
4		1-Hexen-3-ol	100	C6H12O	004798-44-1	37
5		1-Hexen-3-ol	100	C6H12O	004798-44-1	37



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Misc : 25.0mL/MSVOA U/WATER
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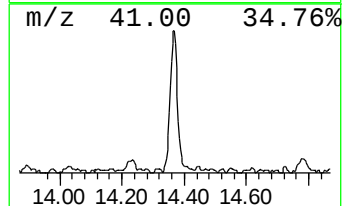
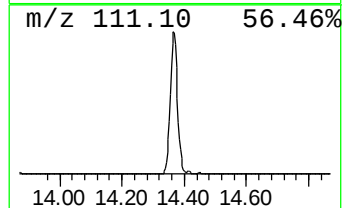
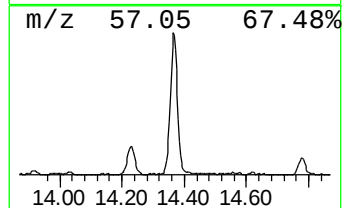
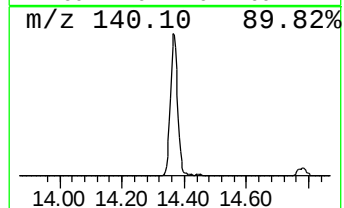
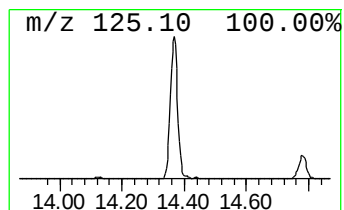
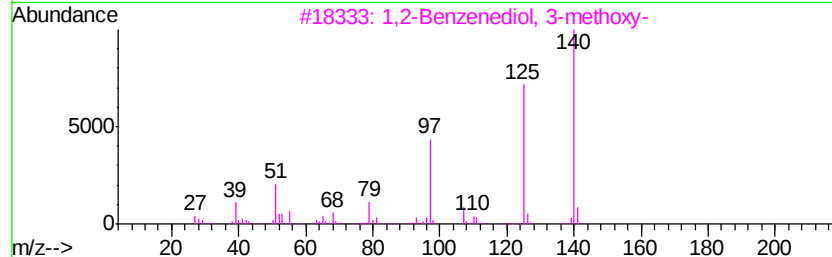
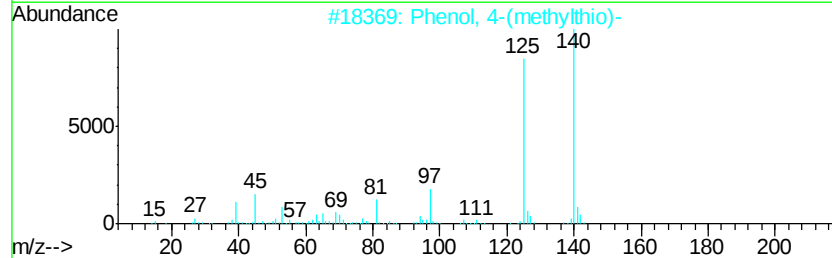
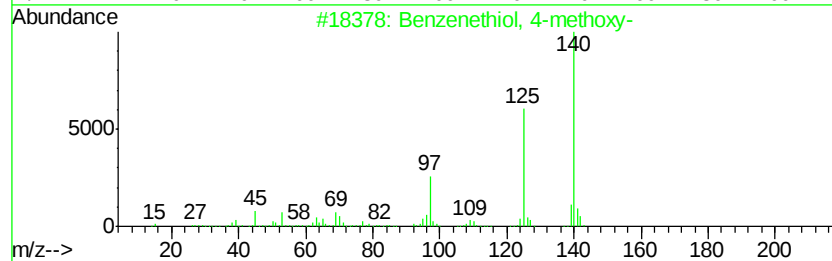
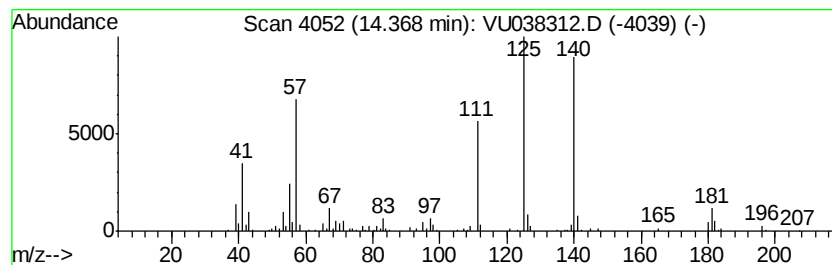
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenethiol, 4-methoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.37	0.95 ug/L	200295	1,4-Dichlorobenzene-d4	11.83
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzenethiol, 4-methoxy-	140 C7H8OS	000696-63-9 58
2		Phenol, 4-(methylthio)-	140 C7H8OS	001073-72-9 58
3		1,2-Benzenediol, 3-methoxy-	140 C7H8O3	000934-00-9 53
4		Uracil, 5-ethyl-	140 C6H8N2O2	004212-49-1 53
5		Phenol, 4-(methylthio)-	140 C7H8OS	001073-72-9 53



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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...	3.22	4.8	ug/L	788055	1	6.28	816378	5.0
Propanal, 2,2-dim...	4.48	11.7	ug/L	1912600	1	6.28	816378	5.0
unknown-01	7.16	8.4	ug/L	1368400	1	6.28	816378	5.0
Benzenethiol, 4-m...	14.37	0.9	ug/L	200295	3	11.83	1057380	5.0