

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU052220\
 Data File : VU038281.D
 Acq On : 22 May 2020 16:43
 Operator : JC/MD
 Sample : L2724-19
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BE4W5

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	1.610	72	84	96	rBV2	177103	303617	15.43%	1.759%
2	1.700	105	112	127	rVB	47631	60924	3.10%	0.353%
3	1.932	175	184	194	rBV	129891	166696	8.47%	0.966%
4	2.594	374	390	400	rBV	256706	430825	21.90%	2.495%
5	2.658	400	410	432	rVB	145794	265213	13.48%	1.536%
6	3.231	566	588	617	rBV2	279282	805444	40.94%	4.665%
7	3.620	694	709	725	rVB3	11400	25841	1.31%	0.150%
8	4.481	953	977	1011	rBV	753388	1967223	100.00%	11.394%
9	4.665	1019	1034	1052	rBV	271541	670619	34.09%	3.884%
10	5.102	1152	1170	1194	rBV	237796	523118	26.59%	3.030%
11	5.424	1255	1270	1284	rBV4	34163	77476	3.94%	0.449%
12	5.758	1350	1374	1409	rBV3	477035	1255704	63.83%	7.273%
13	6.279	1517	1536	1565	rVV	417527	833951	42.39%	4.830%
14	6.420	1569	1580	1595	rVV2	32887	66514	3.38%	0.385%
15	6.719	1659	1673	1691	rBV	303581	591937	30.09%	3.429%
16	7.157	1787	1809	1817	rBV	743476	1520744	77.30%	8.808%
17	7.591	1931	1944	1963	rBV	161235	278024	14.13%	1.610%
18	7.922	2033	2047	2062	rBV	579788	1060185	53.89%	6.141%
19	7.989	2063	2068	2081	rVV	41524	74504	3.79%	0.432%
20	8.202	2121	2134	2145	rBV	105625	181186	9.21%	1.049%
21	8.443	2198	2209	2216	rBV4	13272	23528	1.20%	0.136%
22	8.491	2216	2224	2239	rVB2	27505	60570	3.08%	0.351%
23	8.655	2262	2275	2287	rBV	845592	1477175	75.09%	8.556%
24	8.806	2312	2322	2331	rBV4	24832	41159	2.09%	0.238%
25	9.436	2505	2518	2555	rVB	581079	1021926	51.95%	5.919%
26	10.359	2795	2805	2816	rBV2	22327	35385	1.80%	0.205%
27	10.462	2828	2837	2848	rVB2	13978	22476	1.14%	0.130%
28	10.771	2919	2933	2946	rBV	244303	389486	19.80%	2.256%
29	10.902	2961	2974	2987	rVB2	56503	91913	4.67%	0.532%
30	11.041	3005	3017	3029	rVB3	13733	25476	1.30%	0.148%
31	11.825	3249	3261	3283	rVB	643293	1079071	54.85%	6.250%
32	12.079	3329	3340	3360	rBV4	15368	36914	1.88%	0.214%
33	12.205	3365	3379	3398	rVV	615745	1003903	51.03%	5.815%
34	12.459	3449	3458	3467	rVB5	12587	20355	1.03%	0.118%

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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

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Title : TRACE VOA SOM01.0

35	12.520	3467	3477	3486	rBV	30145	47809	2.43%	0.277%
36	12.799	3552	3564	3573	rBV2	33772	57897	2.94%	0.335%
37	12.909	3586	3598	3612	rVB4	22348	37314	1.90%	0.216%
38	14.115	3961	3973	3984	rBV	83993	135580	6.89%	0.785%
39	14.356	4036	4048	4062	rBV2	131168	208871	10.62%	1.210%
40	14.764	4163	4175	4187	rBV4	12614	21584	1.10%	0.125%
41	15.092	4266	4277	4289	rBV2	57809	95724	4.87%	0.554%
42	15.751	4469	4482	4499	rBV3	77558	145822	7.41%	0.845%
43	16.758	4787	4795	4804	rBV5	15505	25009	1.27%	0.145%

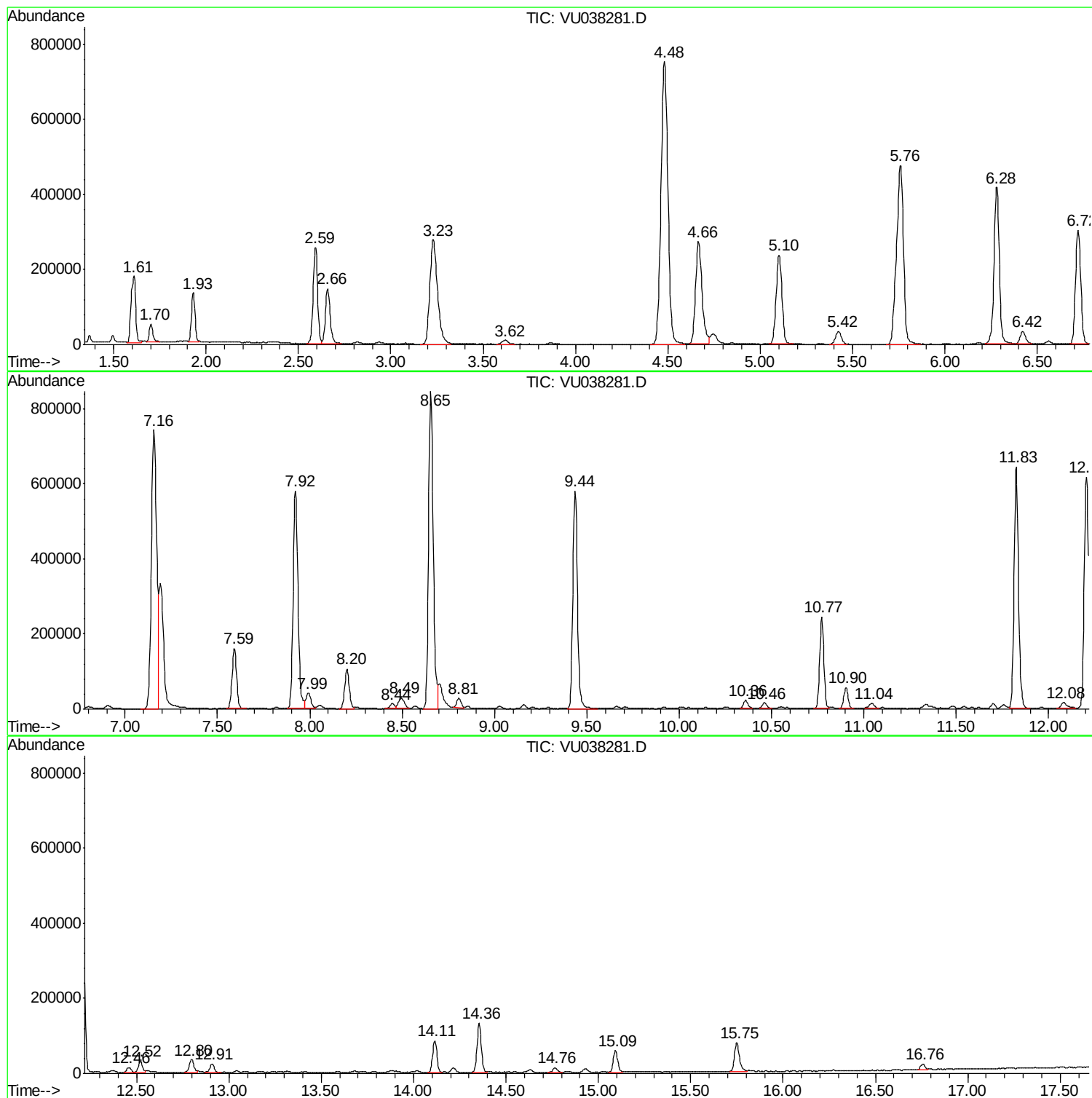
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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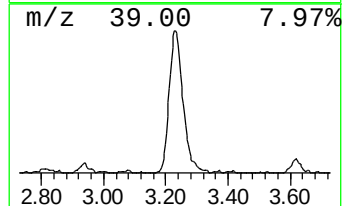
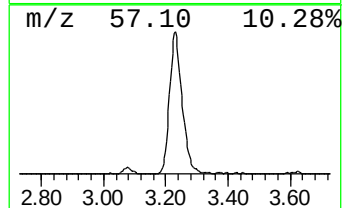
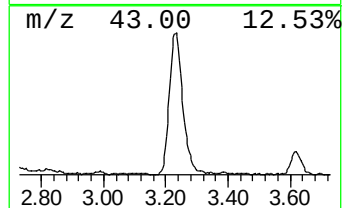
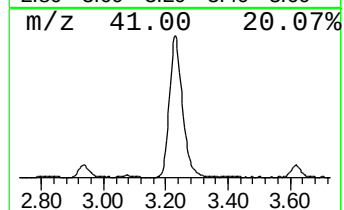
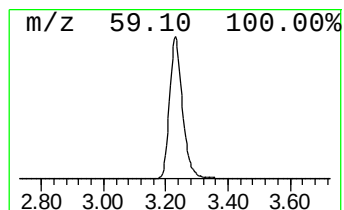
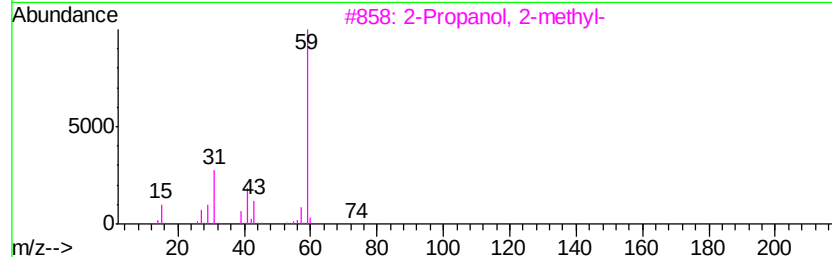
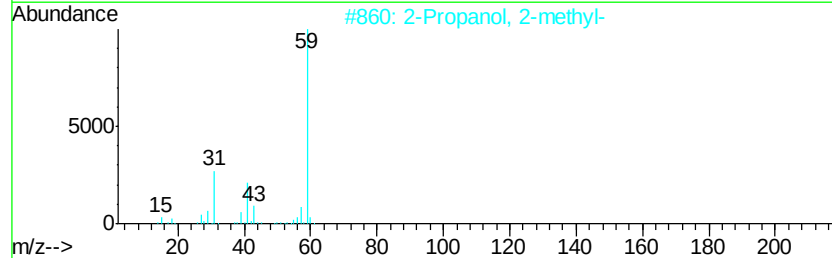
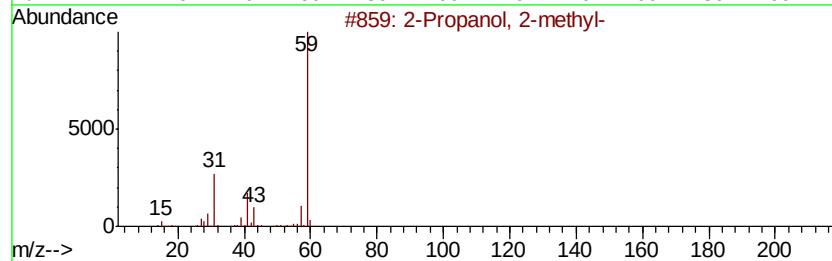
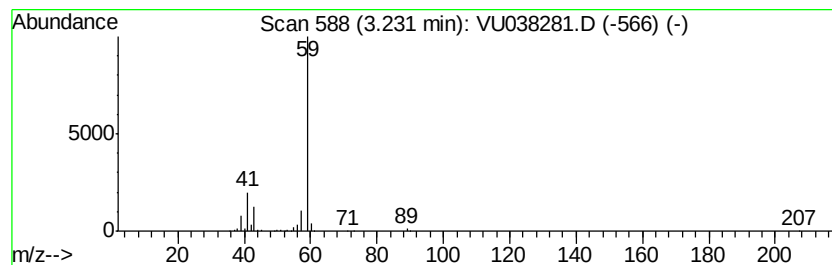
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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.
3.23	4.83 ug/L	805444	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			1,2-Butanediol	90	C4H10O2	000584-03-2	9



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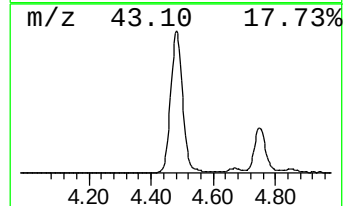
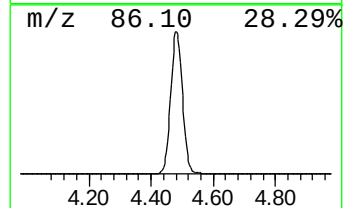
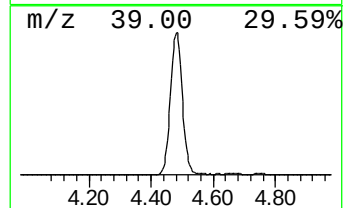
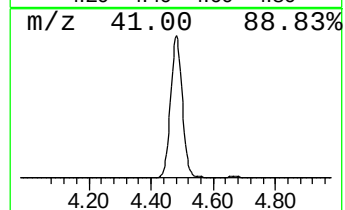
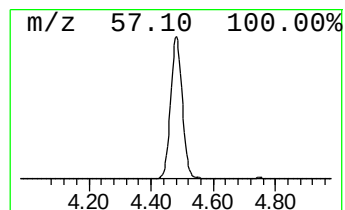
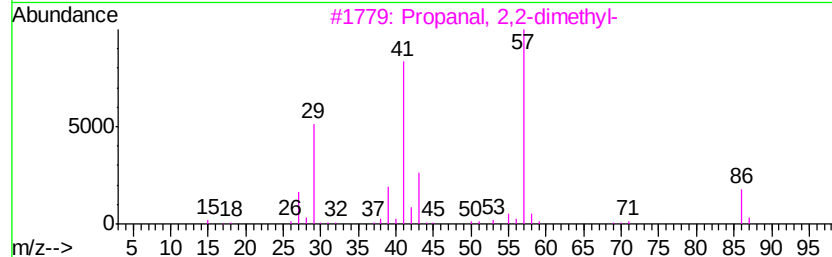
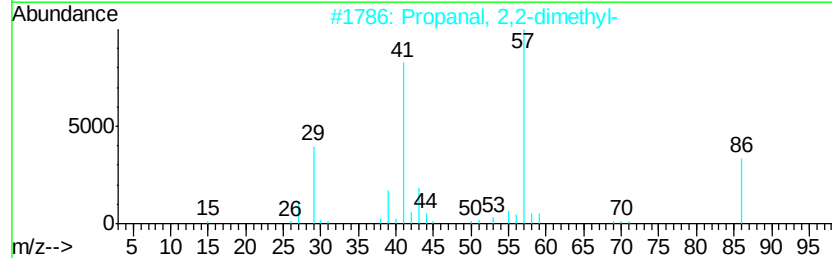
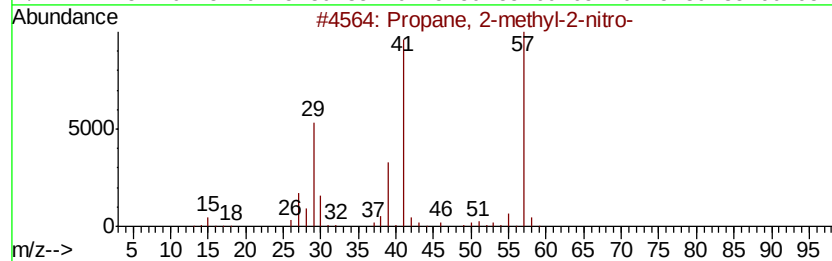
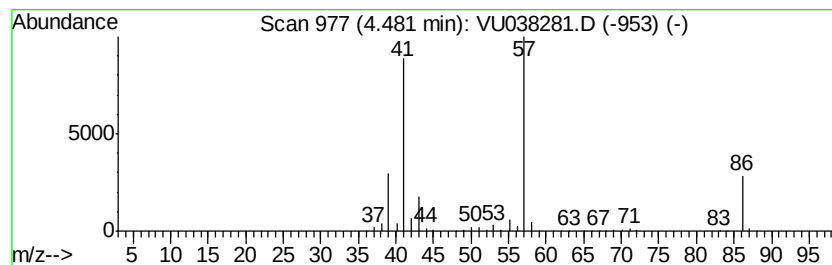
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Quant Title : TRACE VOA SOM01.0

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	11.79 ug/L	1967220	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	50
2		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
3		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	43
5		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	42



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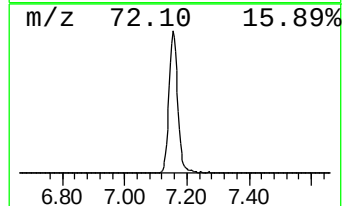
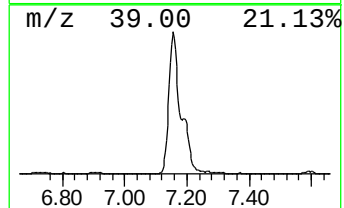
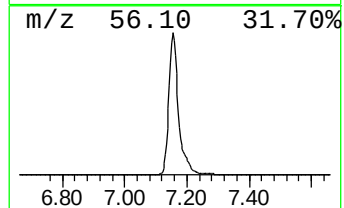
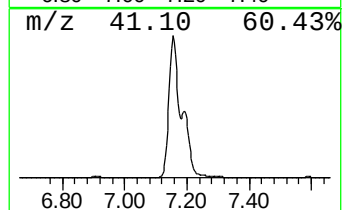
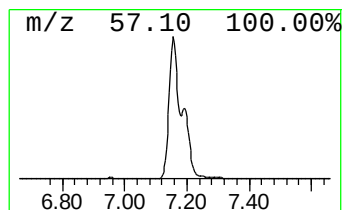
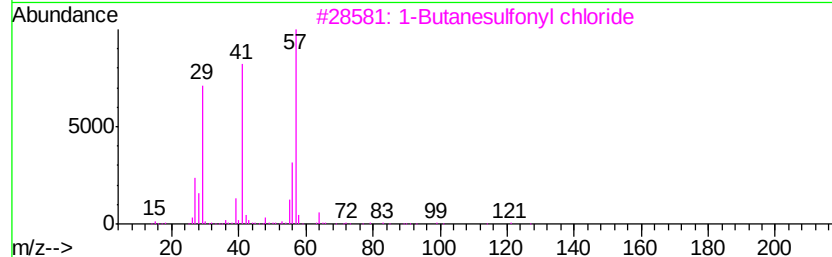
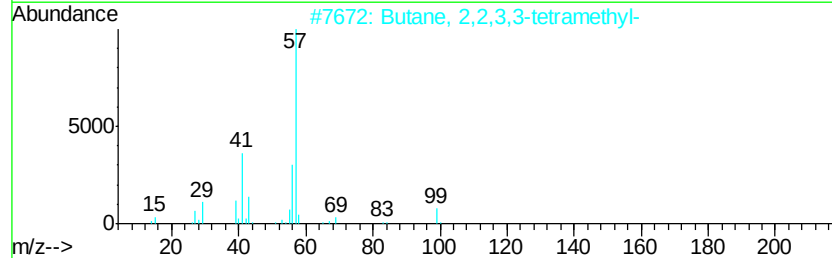
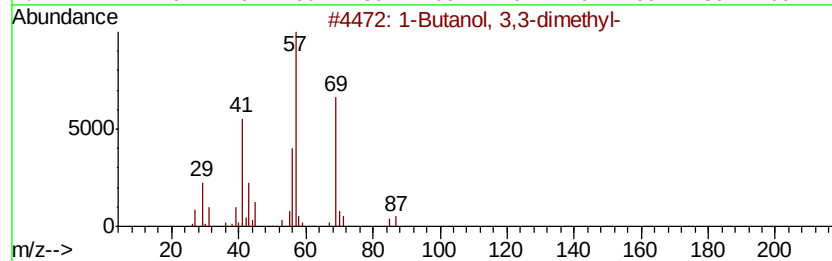
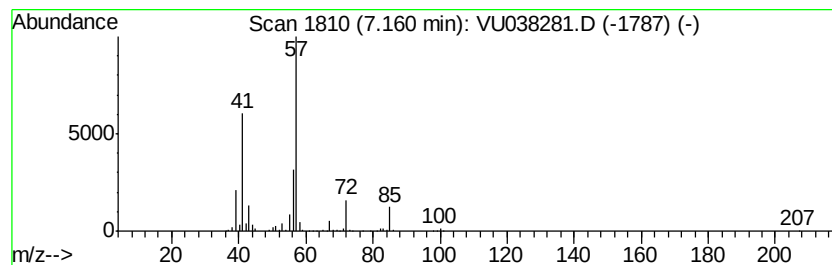
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	9.12 ug/L	1520740	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol, 3,3-dimethyl-	102	C6H14O	000624-95-3	40
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
3		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
4		3,4-Hexanedione, 2,2,5,5-tetrame...	185	C10H19NO2	039950-93-1	37
5		Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	37



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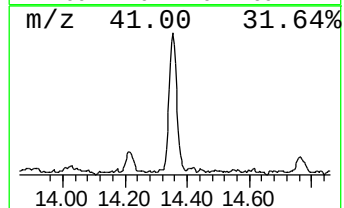
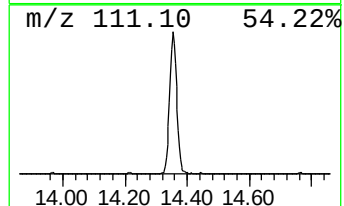
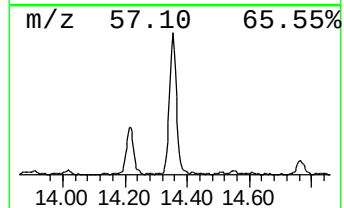
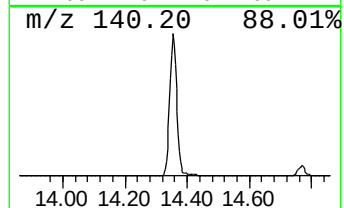
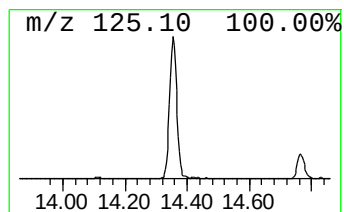
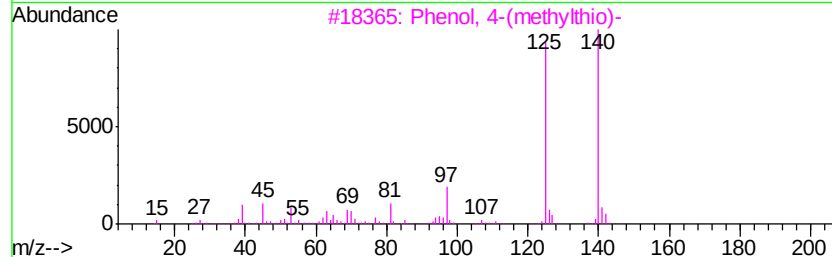
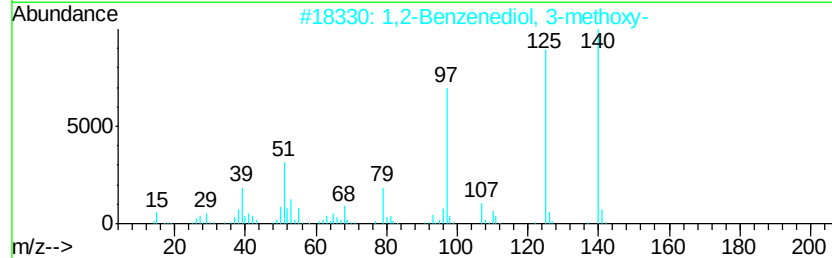
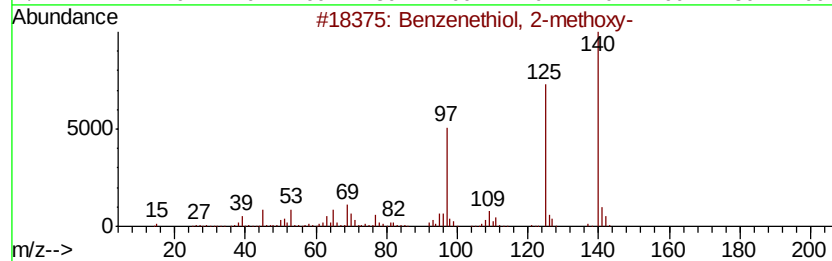
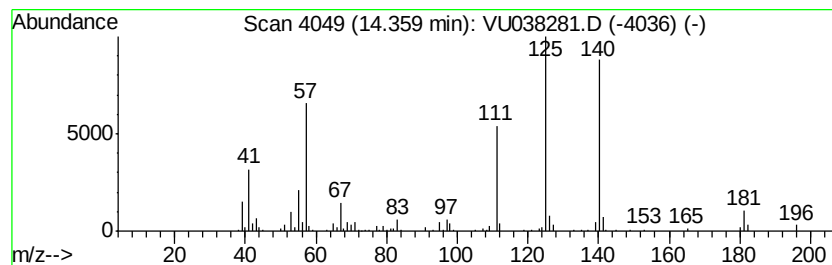
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.36	0.97 ug/L	208871	1,4-Dichlorobenzene-d4	11.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	64
2	1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
3	Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
4	2-Methoxyresorcinol	140	C7H8O3	029267-67-2	53
5	3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	53



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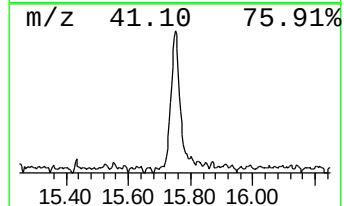
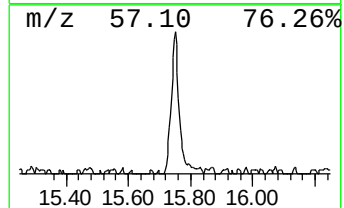
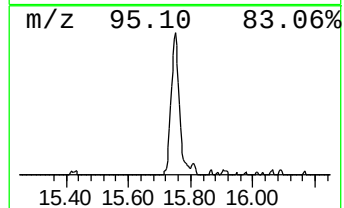
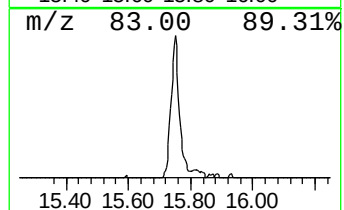
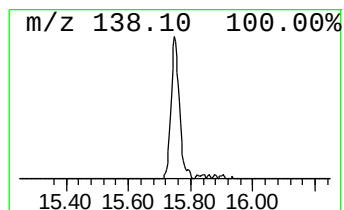
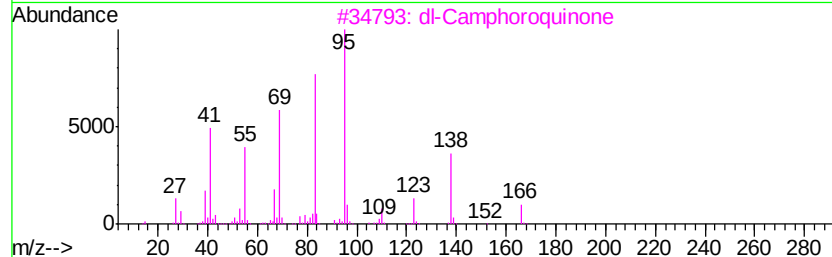
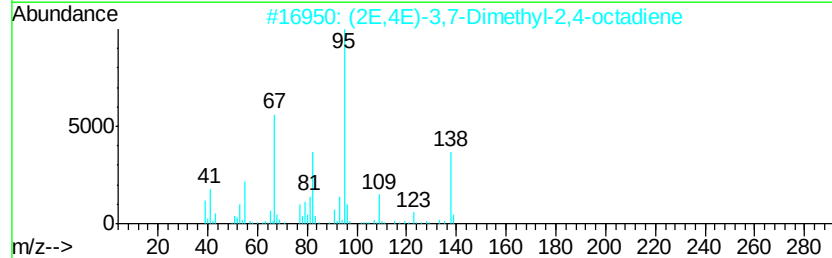
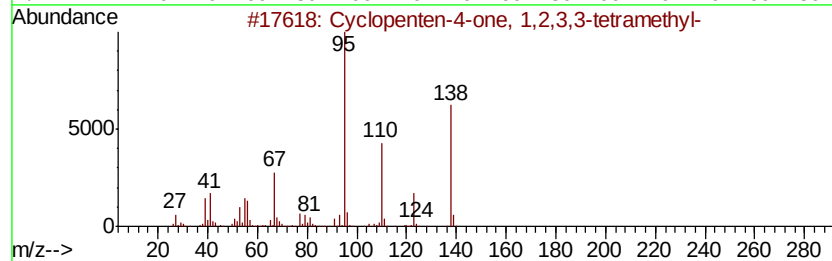
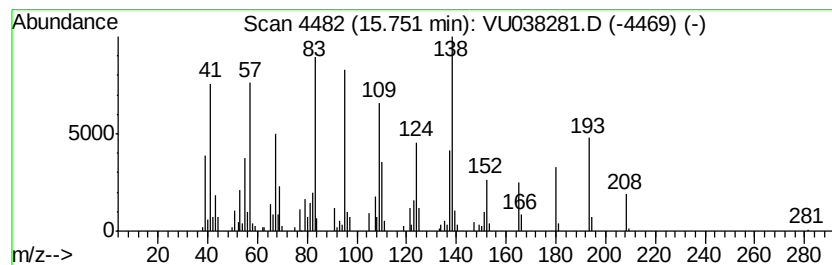
Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.75	0.68 ug/L	145822	1,4-Dichlorobenzene-d4	11.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopenten-4-one, 1,2,3,3-tetra...	138	C9H14O	1000163-38-6	38
2	(2E,4E)-3,7-Dimethyl-2,4-octadiene	138	C10H18	1000374-08-2	30
3	dl-Camphoroquinone	166	C10H14O2	010373-78-1	30
4	(2Z,4E)-3,7-Dimethyl-2,4-octadiene	138	C10H18	1000374-08-4	25
5	Pyrazine, 2-methoxy-3-(1-methylp...	166	C9H14N2O	024168-70-5	25



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU052220\
Data File : VU038281.D
Acq On : 22 May 2020 16:43
Operator : JC/MD
Sample : L2724-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BE4W5

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...	3.23	4.8	ug/L	805444	1	6.28	833951	5.0
Propane, 2-methyl...	4.48	11.8	ug/L	1967220	1	6.28	833951	5.0
unknown-01	7.16	9.1	ug/L	1520740	1	6.28	833951	5.0
Benzenethiol, 2-m...	14.36	1.0	ug/L	208871	3	11.83	1079070	5.0
unknown-02	15.75	0.7	ug/L	145822	3	11.83	1079070	5.0