

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
 Data File : VU038954.D
 Acq On : 17 Jun 2020 19:12
 Operator : SY/MD
 Sample : L3040-10
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9L23

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\SOMUTR061720WMA.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	1.620	76	87	96	rBV	134564	162788	11.63%	1.529%
2	1.752	120	128	138	rVB3	14285	24698	1.77%	0.232%
3	1.945	180	188	200	rBV	107783	146107	10.44%	1.373%
4	2.597	381	391	404	rVB	312297	492867	35.22%	4.630%
5	2.819	454	460	471	rVB3	19450	31126	2.22%	0.292%
6	2.932	490	495	499	rBV2	12730	17041	1.22%	0.160%
7	4.527	969	991	1011	rBV8	21435	69001	4.93%	0.648%
8	4.774	1034	1068	1116	rBV	112158	526414	37.62%	4.945%
9	5.137	1163	1181	1201	rBV	205231	459091	32.81%	4.313%
10	5.793	1363	1385	1412	rBV2	444814	1066754	76.24%	10.022%
11	6.308	1532	1545	1563	rVB	345385	632665	45.21%	5.944%
12	6.687	1653	1663	1668	rBV5	10616	17679	1.26%	0.166%
13	6.745	1669	1681	1701	rVB	264081	510274	36.47%	4.794%
14	7.224	1820	1830	1844	rVB2	34429	71394	5.10%	0.671%
15	7.607	1935	1949	1962	rBV2	130211	224178	16.02%	2.106%
16	7.842	2009	2022	2029	rBV5	7158	14855	1.06%	0.140%
17	7.935	2038	2051	2065	rVB	452610	776993	55.53%	7.299%
18	8.214	2126	2138	2151	rBV	85751	141533	10.11%	1.330%
19	8.671	2260	2280	2315	rBV	770801	1399265	100.00%	13.145%
20	8.816	2318	2325	2336	rVB3	13150	20496	1.46%	0.193%
21	9.440	2507	2519	2538	rBV	485655	804901	57.52%	7.562%
22	9.661	2582	2588	2597	rVB2	10755	15330	1.10%	0.144%
23	9.790	2612	2628	2643	rBV6	8880	20165	1.44%	0.189%
24	10.362	2797	2806	2819	rBV5	16848	26377	1.89%	0.248%
25	10.774	2921	2934	2946	rBV	217129	342525	24.48%	3.218%
26	11.063	3013	3024	3033	rVB4	8840	15732	1.12%	0.148%
27	11.700	3213	3222	3230	rBV3	16901	23376	1.67%	0.220%
28	11.825	3249	3261	3276	rVB	491229	766640	54.79%	7.202%
29	12.076	3327	3339	3360	rBV2	38488	81070	5.79%	0.762%
30	12.205	3366	3379	3392	rVB	499930	792303	56.62%	7.443%
31	12.337	3411	3420	3431	rBV2	13895	21822	1.56%	0.205%
32	12.790	3551	3561	3571	rBV3	18302	28882	2.06%	0.271%
33	12.906	3587	3597	3607	rBV5	25628	41251	2.95%	0.388%
34	14.015	3932	3942	3952	rBV5	14100	22806	1.63%	0.214%

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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\SOMUTR061720WMA.M
Title : TRACE VOA SOM01.0

35	14.227	3997	4008	4019	rBV3	90925	141414	10.11%	1.329%
36	14.349	4038	4046	4057	rVB5	9381	15395	1.10%	0.145%
37	14.700	4141	4155	4167	rBV5	7162	18859	1.35%	0.177%
38	14.873	4199	4209	4217	rBV3	12805	28351	2.03%	0.266%
39	14.918	4218	4223	4232	rVB8	10073	17297	1.24%	0.162%
40	15.044	4252	4262	4271	rBV5	9820	18118	1.29%	0.170%
41	15.742	4470	4479	4493	rVB5	36384	59963	4.29%	0.563%
42	16.192	4612	4619	4626	rVB7	12333	19243	1.38%	0.181%
43	16.835	4810	4819	4829	rBV4	37614	59526	4.25%	0.559%
44	16.963	4846	4859	4876	rBV	264820	458061	32.74%	4.303%

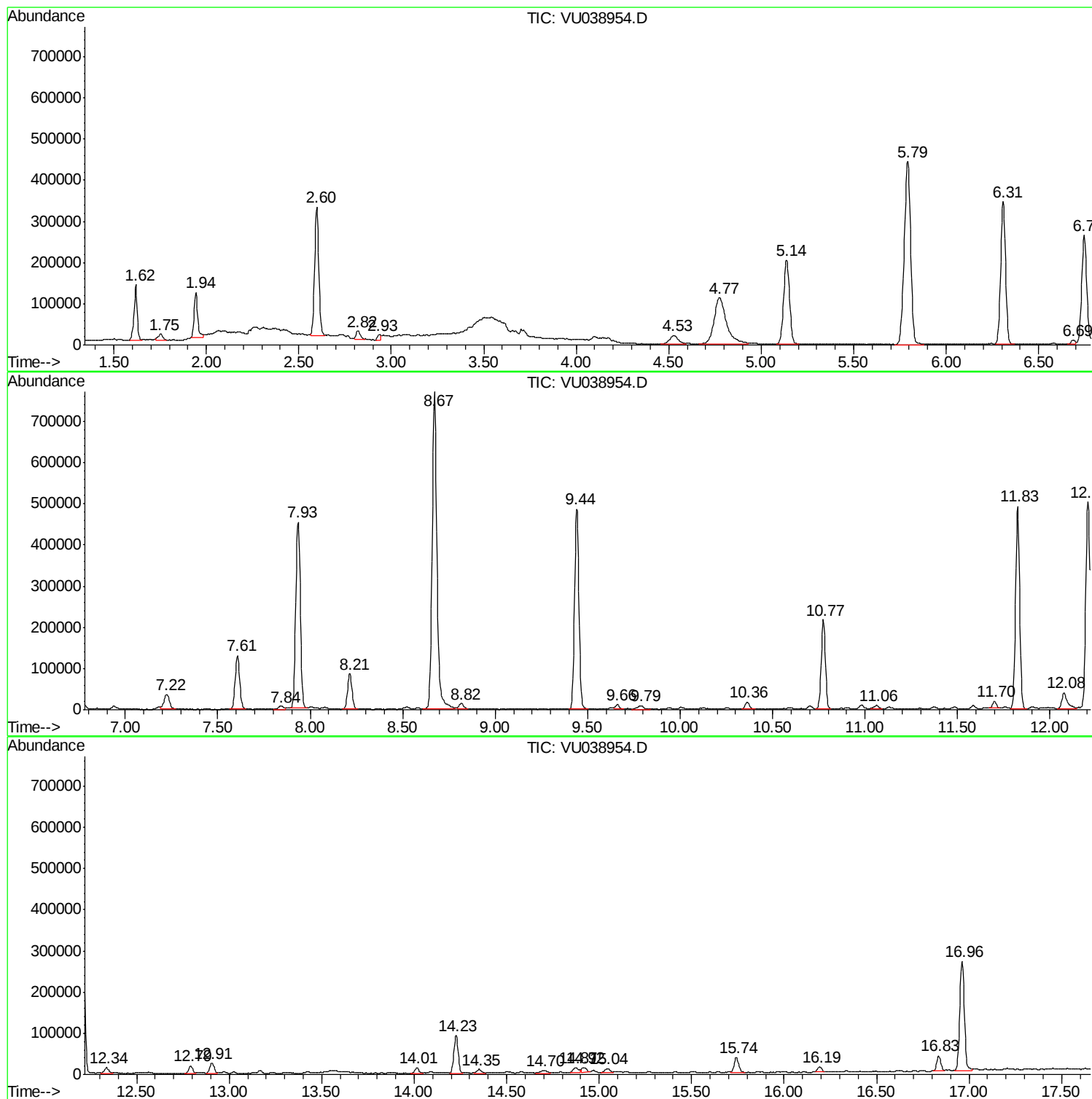
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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ALS Vial : 1 Sample Multiplier: 1

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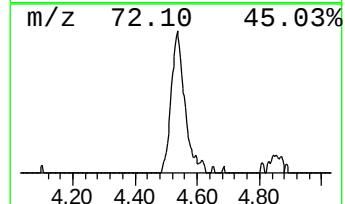
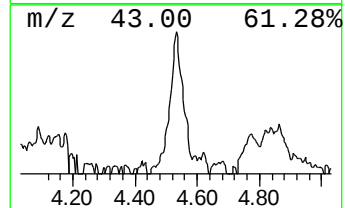
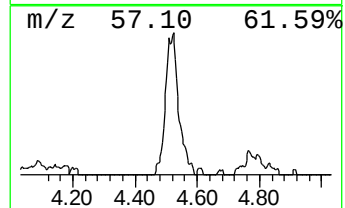
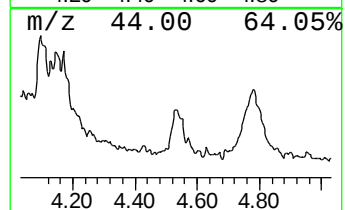
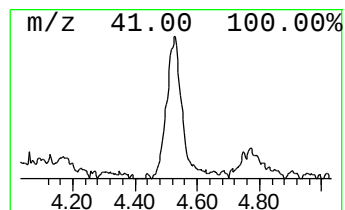
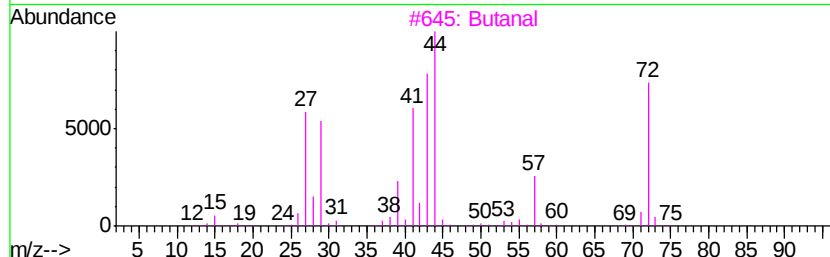
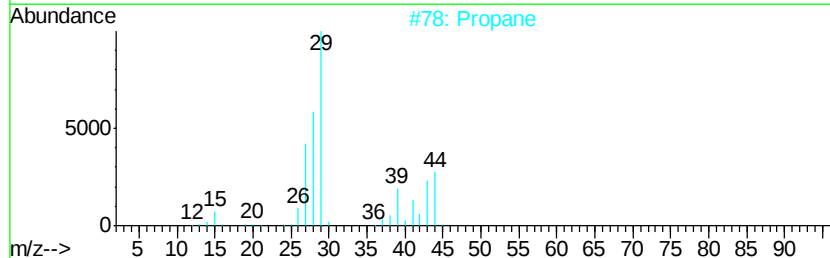
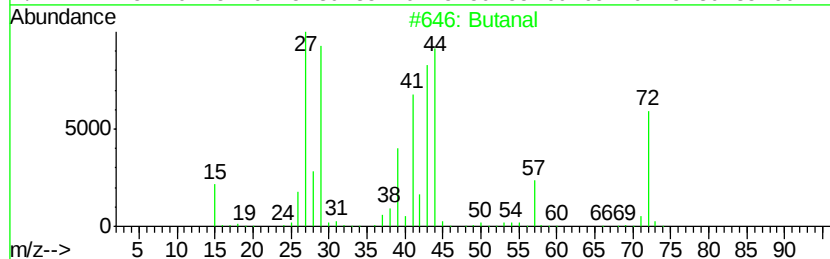
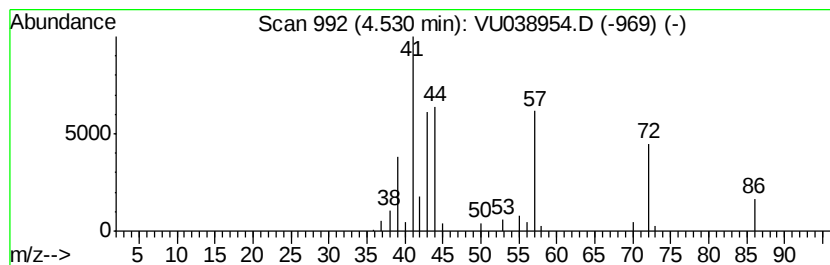
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	0.55 ug/L	69001	1,4-Difluorobenzene	6.31

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal		72	C4H8O	000123-72-8	50
2	Propane		44	C3H8	000074-98-6	43
3	Butanal		72	C4H8O	000123-72-8	38
4	Butanal		72	C4H8O	000123-72-8	38
5	Cyclopropanecarboxamide		85	C4H7NO	006228-73-5	38



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Instrument :
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ClientSampleId :
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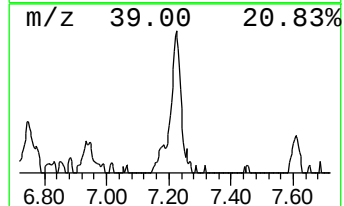
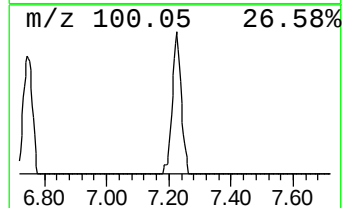
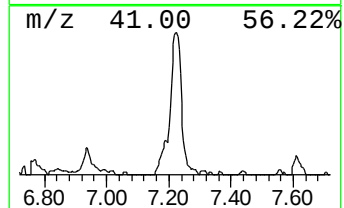
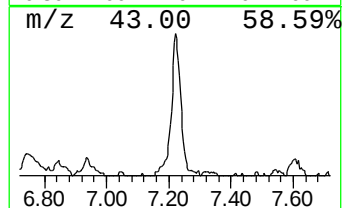
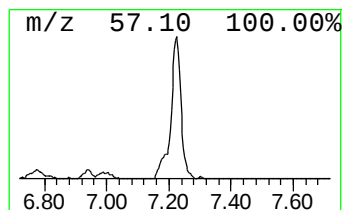
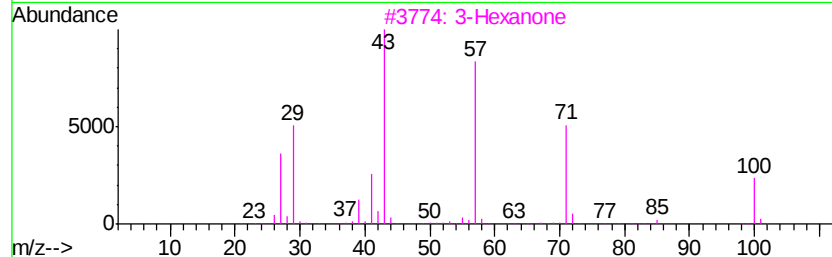
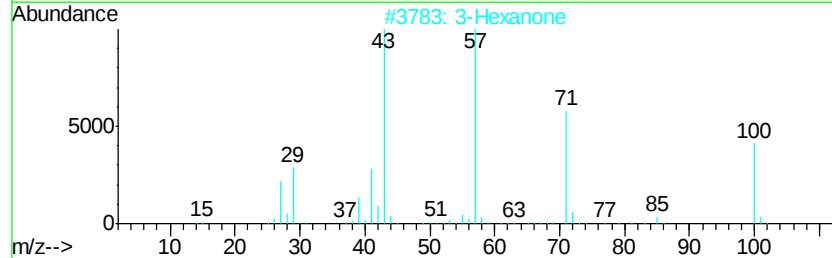
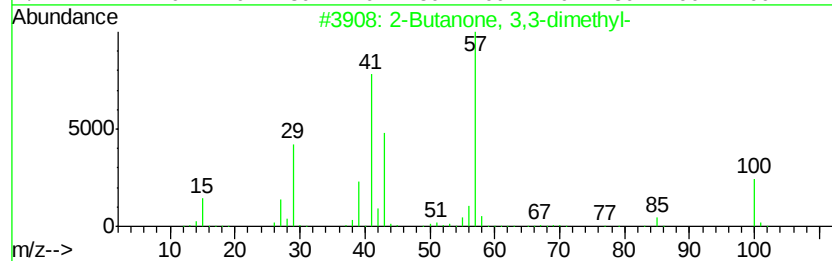
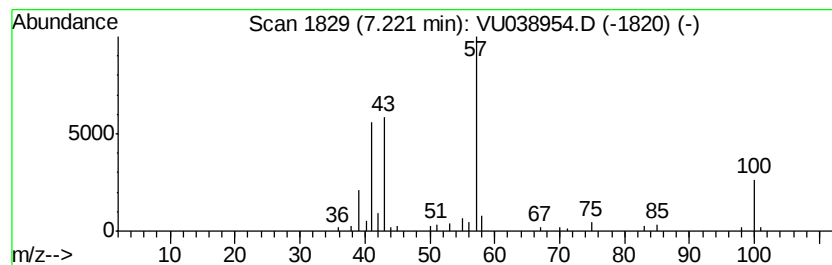
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	0.56 ug/L	71394	1,4-Difluorobenzene	6.31

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
2			3-Hexanone	100	C6H12O	000589-38-8	64
3			3-Hexanone	100	C6H12O	000589-38-8	59
4			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	53
5			3-Hexanone	100	C6H12O	000589-38-8	50



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

Instrument :
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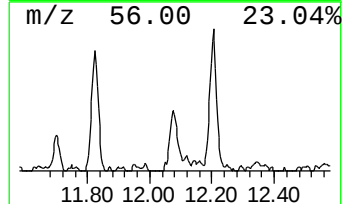
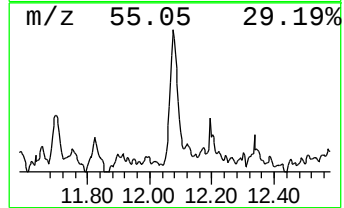
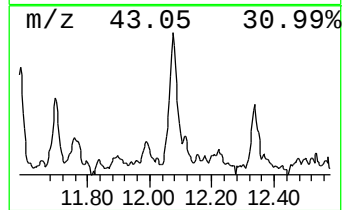
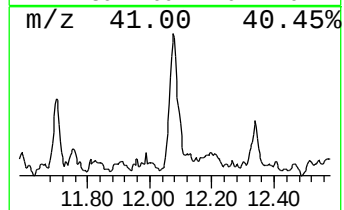
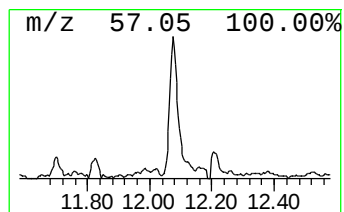
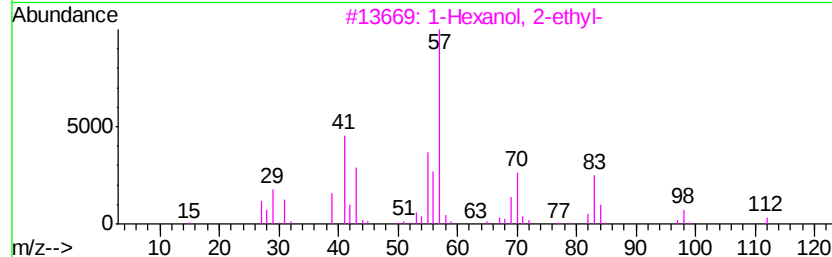
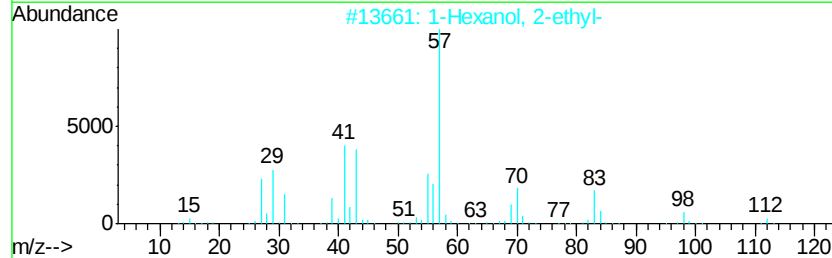
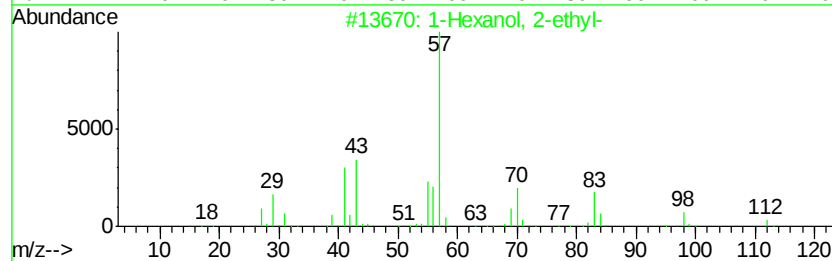
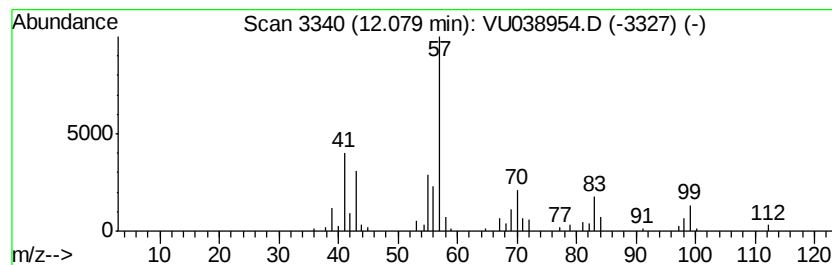
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	0.53 ug/L	81070	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
5		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59



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

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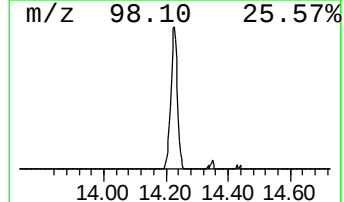
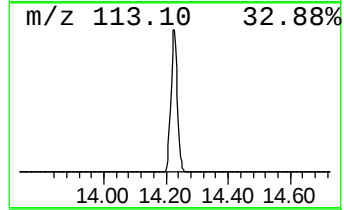
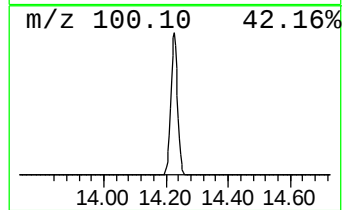
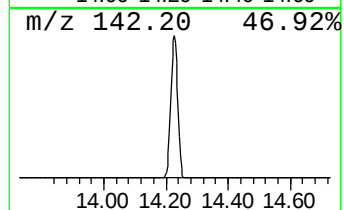
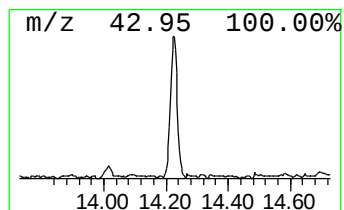
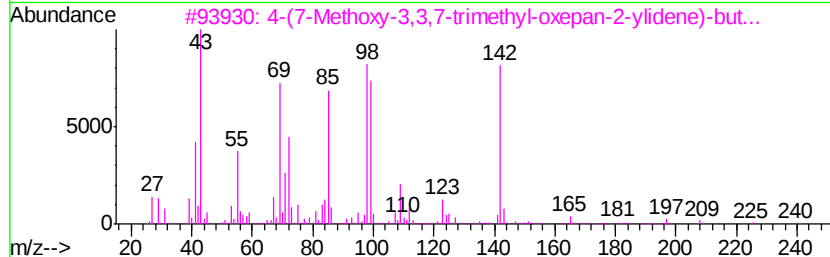
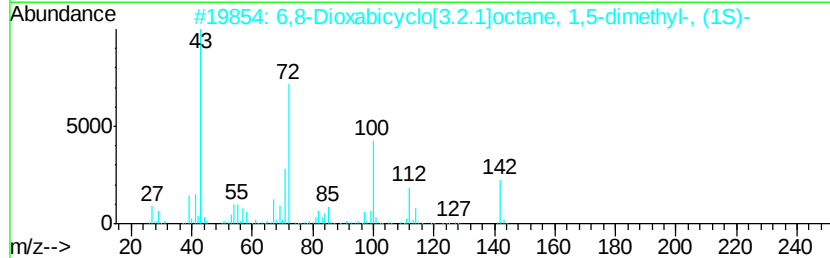
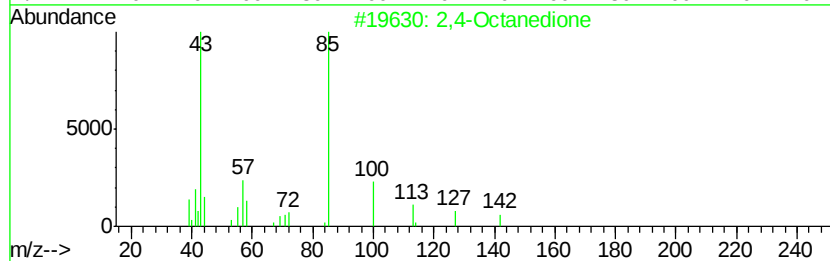
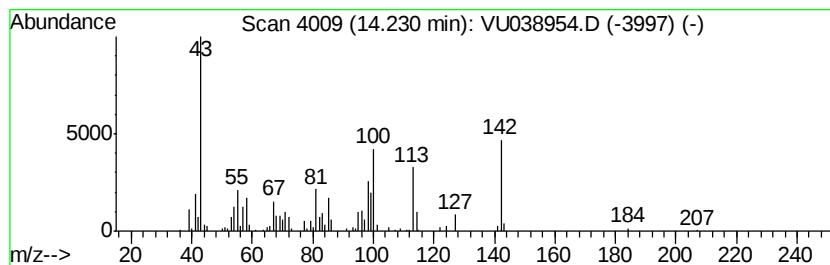
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	0.92 ug/L	141414	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Octanedione	142	C8H14O2	014090-87-0	47
2		6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	27
3		4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	16
4		6-Dodecanone	184	C12H24O	006064-27-3	12
5		4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	12



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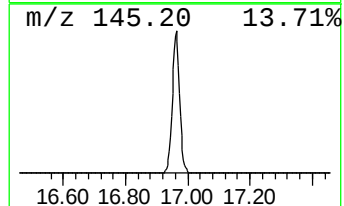
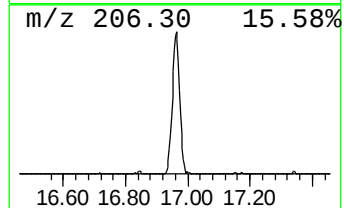
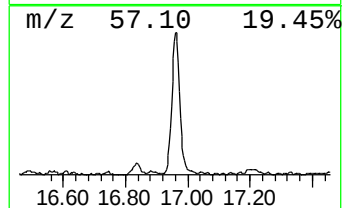
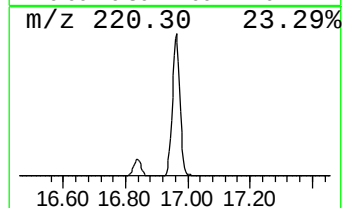
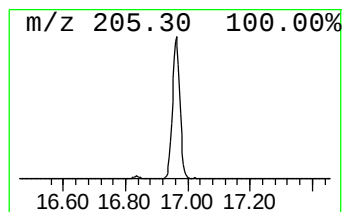
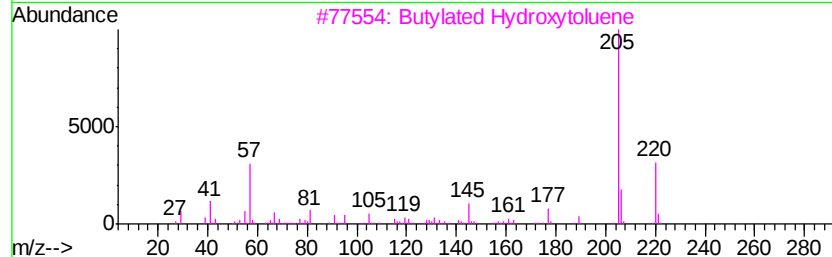
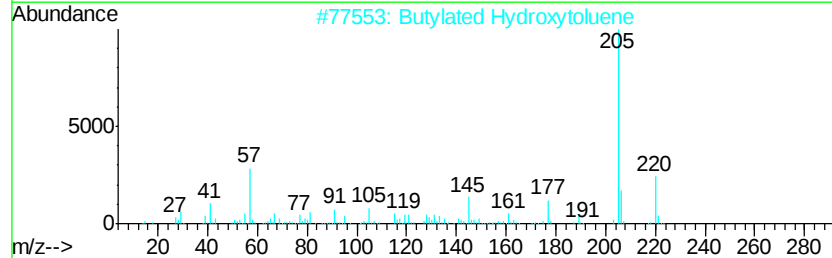
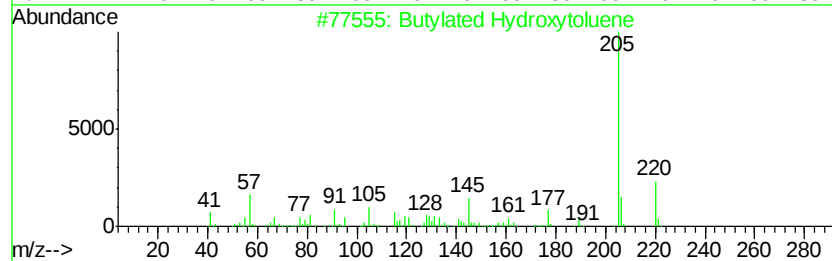
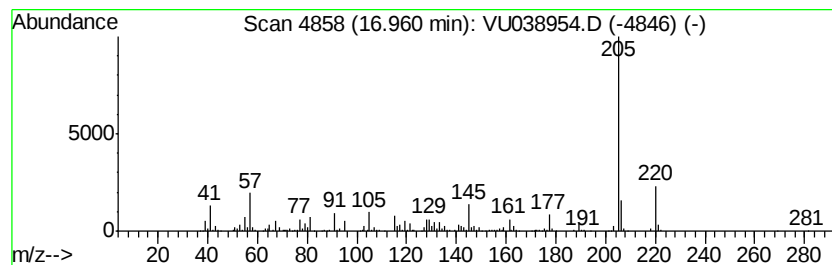
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	2.99 ug/L	458061	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	99
2	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	98
3	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	96
4	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 2,4,6-tris(1-methylethyl)-		220	C15H24O	002934-07-8	87



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038954.D
Acq On : 17 Jun 2020 19:12
Operator : SY/MD
Sample : L3040-10
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L23

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.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
Butanal	4.53	0.6	ug/L	69001	1	6.31	632665	5.0
2-Butanone, 3,3-d...	7.22	0.6	ug/L	71394	1	6.31	632665	5.0
1-Hexanol, 2-ethyl-	12.08	0.5	ug/L	81070	3	11.83	766640	5.0
unknown-01	14.23	0.9	ug/L	141414	3	11.83	766640	5.0
Butylated Hydroxy...	16.96	3.0	ug/L	458061	3	11.83	766640	5.0