

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
 Data File : VU038951.D
 Acq On : 17 Jun 2020 18:02
 Operator : SY/MD
 Sample : L3040-07
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9L17

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	1.629	79	90	101	rBV	131151	162603	6.17%	1.177%
2	1.951	183	190	202	rBV	103457	130677	4.96%	0.946%
3	2.607	384	394	416	rVB	296436	502718	19.07%	3.637%
4	2.800	445	454	458	rBV3	18305	34352	1.30%	0.249%
5	4.530	973	992	996	rBV9	10653	28378	1.08%	0.205%
6	4.806	1046	1078	1119	rBV	92614	485969	18.43%	3.516%
7	5.163	1172	1189	1207	rBV	206563	449965	17.07%	3.256%
8	5.803	1363	1388	1415	rBV2	422237	1016197	38.55%	7.353%
9	6.317	1534	1548	1570	rVB	334402	625358	23.72%	4.525%
10	6.751	1671	1683	1702	rVB	249280	475906	18.05%	3.443%
11	6.851	1705	1714	1728	rVB2	13380	28106	1.07%	0.203%
12	7.230	1808	1832	1845	rBV3	33143	75721	2.87%	0.548%
13	7.610	1938	1950	1970	rVB	124242	212152	8.05%	1.535%
14	7.938	2040	2052	2068	rVB	444078	751333	28.50%	5.436%
15	8.217	2124	2139	2151	rBV	85256	142459	5.40%	1.031%
16	8.674	2264	2281	2292	rBV	706466	1272670	48.28%	9.209%
17	9.443	2507	2520	2541	rBV	485073	799583	30.33%	5.785%
18	9.661	2580	2588	2600	rVB2	22878	36496	1.38%	0.264%
19	9.799	2613	2631	2644	rBV5	16270	39426	1.50%	0.285%
20	9.941	2661	2675	2688	rBV3	45646	76681	2.91%	0.555%
21	10.150	2733	2740	2755	rVB2	17163	29599	1.12%	0.214%
22	10.256	2755	2773	2784	rBV	51107	93075	3.53%	0.673%
23	10.365	2799	2807	2829	rVB7	13255	32335	1.23%	0.234%
24	10.703	2904	2912	2922	rVB2	27060	42872	1.63%	0.310%
25	10.774	2922	2934	2947	rBV	211114	338672	12.85%	2.450%
26	10.983	2988	2999	3013	rVB	46888	76817	2.91%	0.556%
27	11.066	3013	3025	3035	rBV6	17035	31671	1.20%	0.229%
28	11.484	3146	3155	3164	rBV3	23406	35527	1.35%	0.257%
29	11.584	3177	3186	3197	rBV3	49826	77261	2.93%	0.559%
30	11.825	3248	3261	3275	rVB	526568	817306	31.00%	5.914%
31	12.076	3323	3339	3368	rBV	1411814	2636258	100.00%	19.075%
32	12.204	3369	3379	3402	rVB	542473	929435	35.26%	6.725%
33	12.793	3552	3562	3572	rBV2	73756	112998	4.29%	0.818%
34	12.909	3590	3598	3610	rVB3	24024	37182	1.41%	0.269%

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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	13.642	3817	3826	3842	rVB3	27976	44050	1.67%	0.319%
36	14.227	3994	4008	4019	rBV	85940	138639	5.26%	1.003%
37	15.745	4470	4480	4490	rVB10	19685	32640	1.24%	0.236%
38	16.195	4609	4620	4630	rBV4	23541	38924	1.48%	0.282%
39	16.838	4810	4820	4832	rBV2	97440	160339	6.08%	1.160%
40	16.963	4846	4859	4875	rBV	453621	768235	29.14%	5.559%

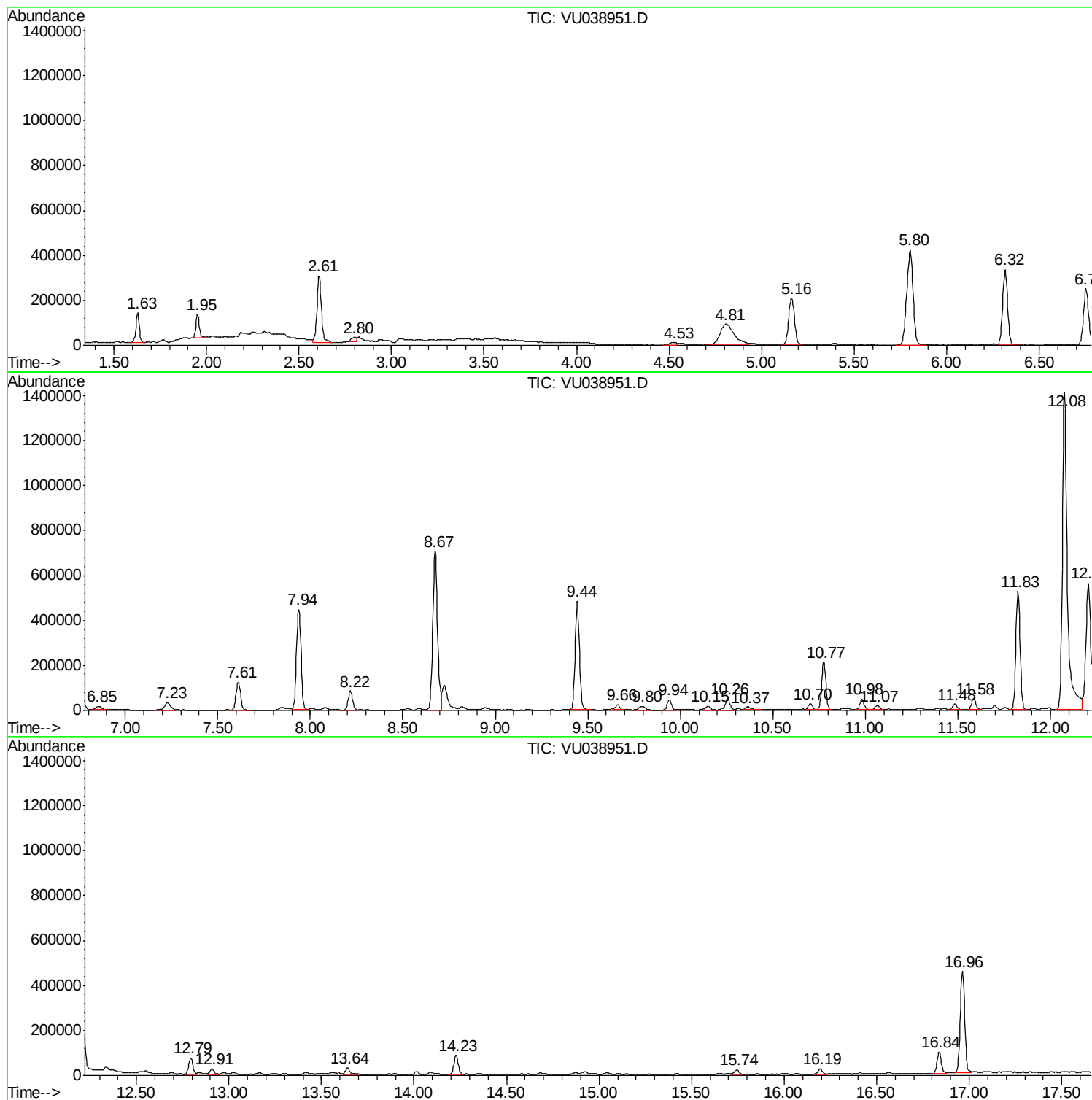
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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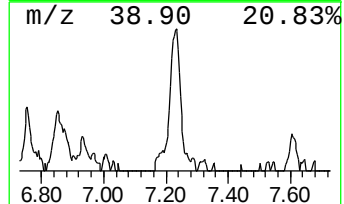
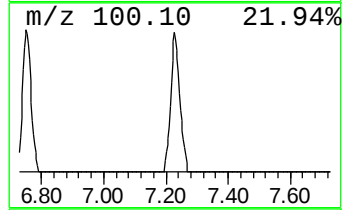
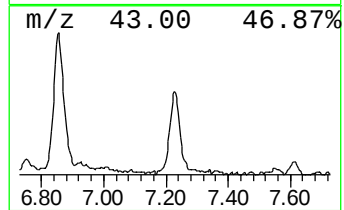
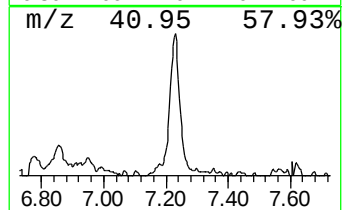
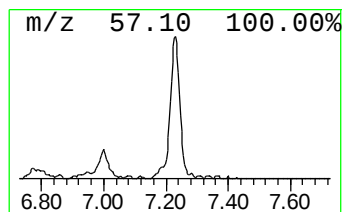
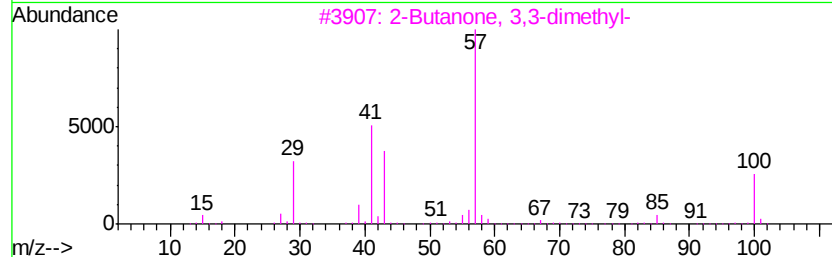
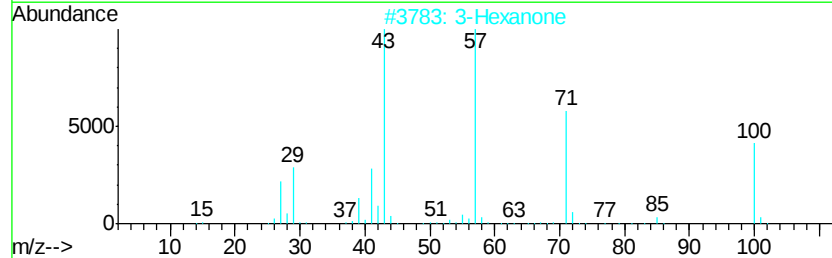
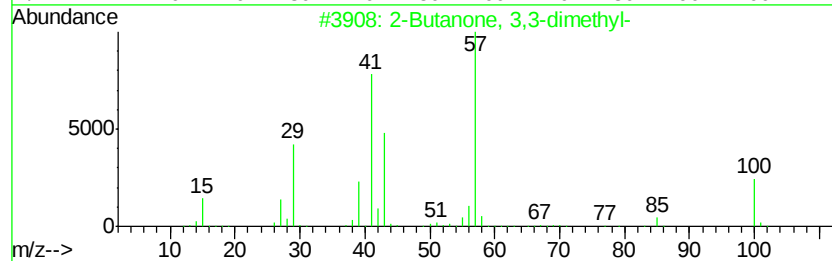
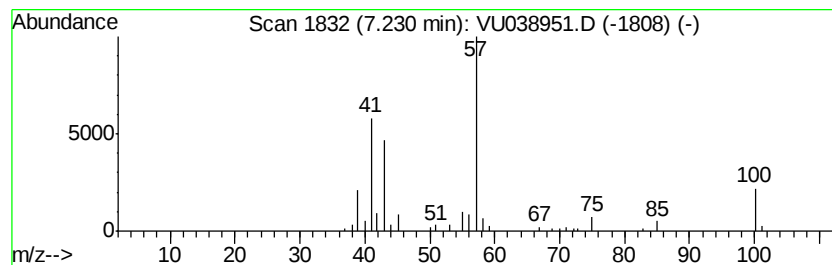
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	0.61 ug/L	75721	1,4-Difluorobenzene	6.32

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72
2			3-Hexanone	100	C6H12O	000589-38-8	64
3			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
4			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	59
5			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	53



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Sample : L3040-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L17

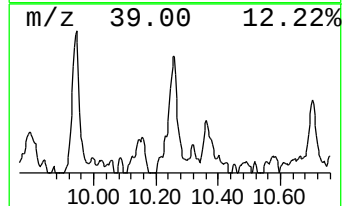
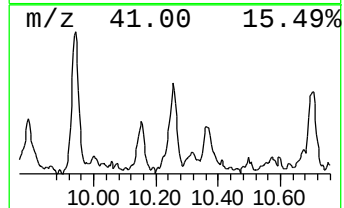
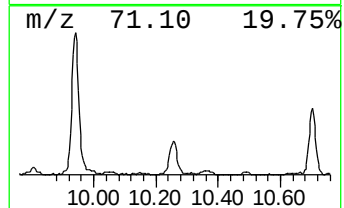
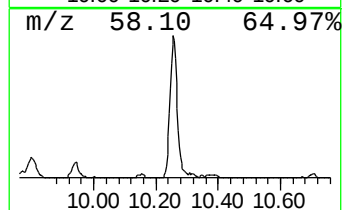
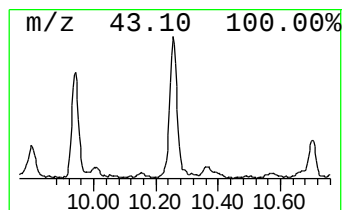
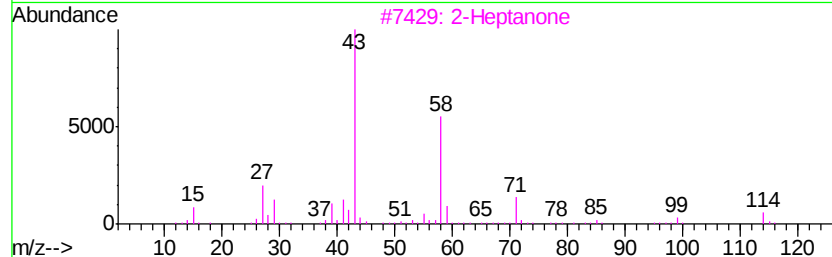
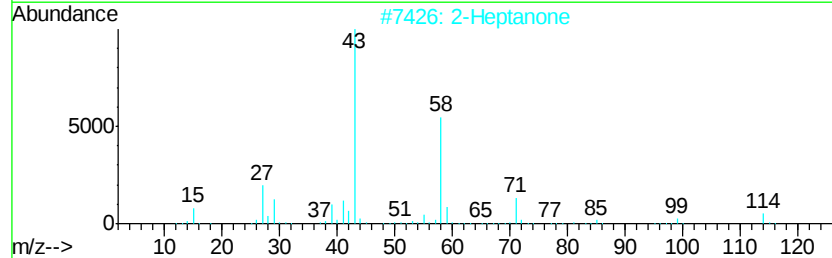
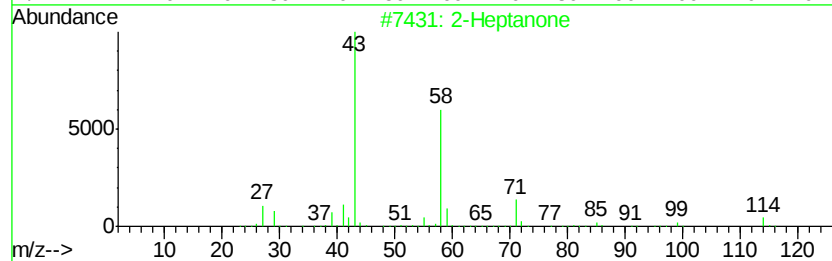
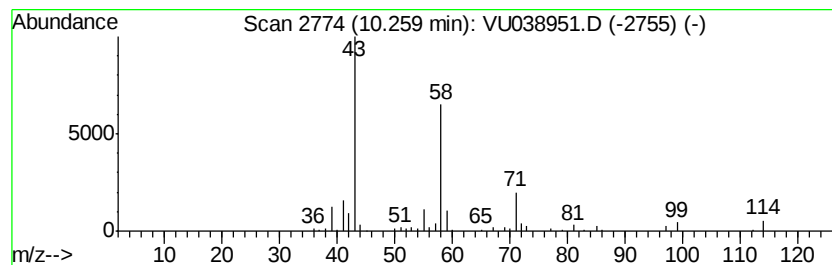
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Heptanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.26	0.58 ug/L	93075	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanone	114	C7H14O	000110-43-0	91
2		2-Heptanone	114	C7H14O	000110-43-0	91
3		2-Heptanone	114	C7H14O	000110-43-0	86
4		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	64
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64



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

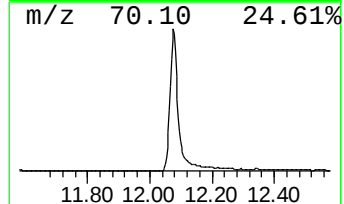
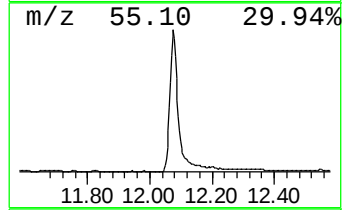
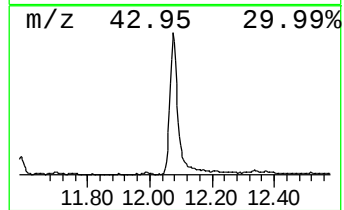
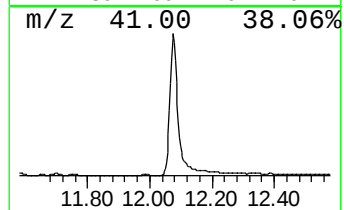
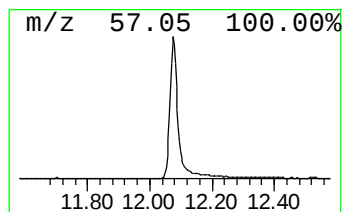
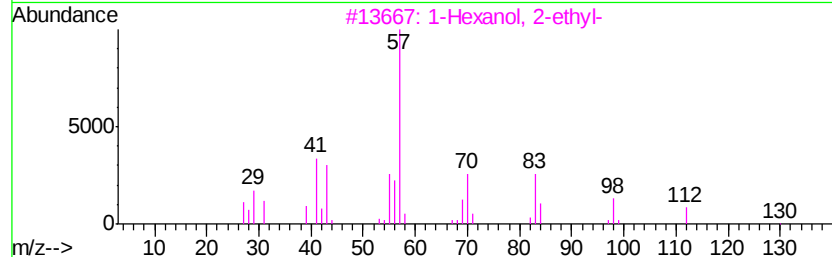
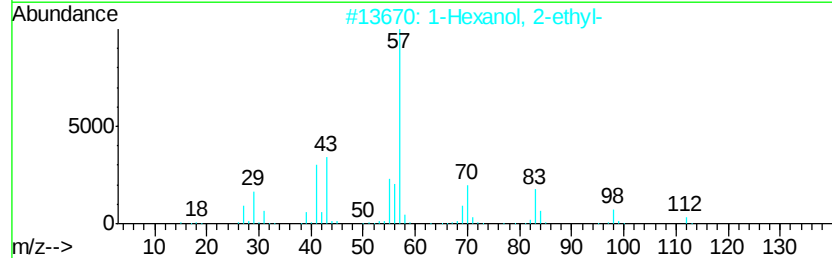
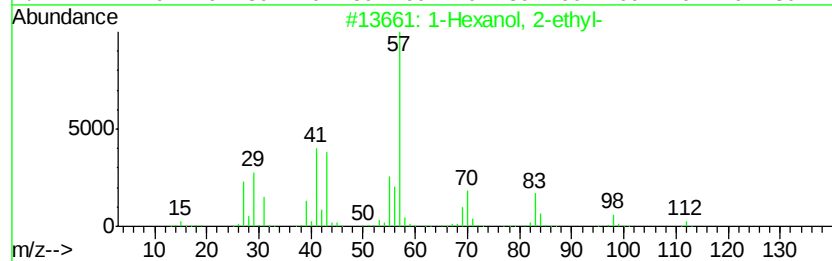
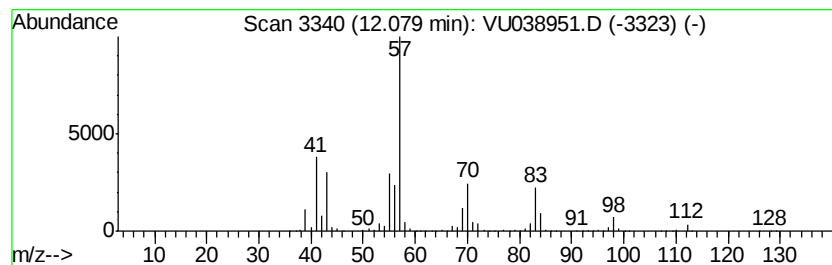
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.08	16.13 ug/L	2636260	1,4-Dichlorobenzene-d4	11.82	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56



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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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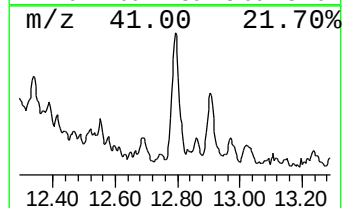
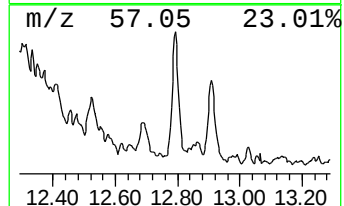
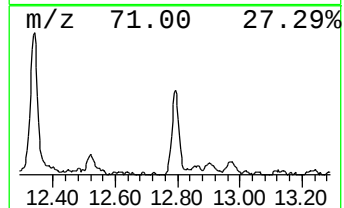
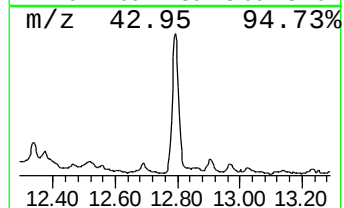
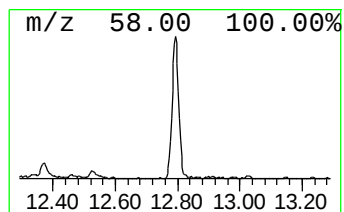
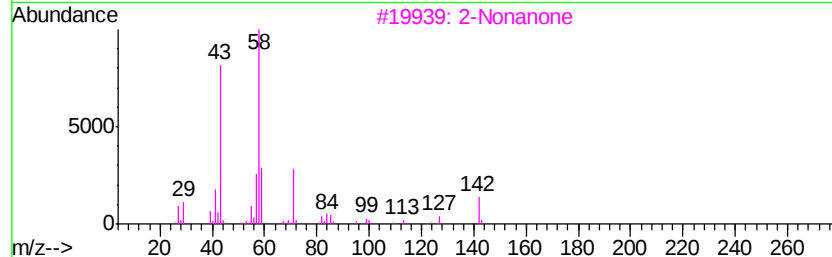
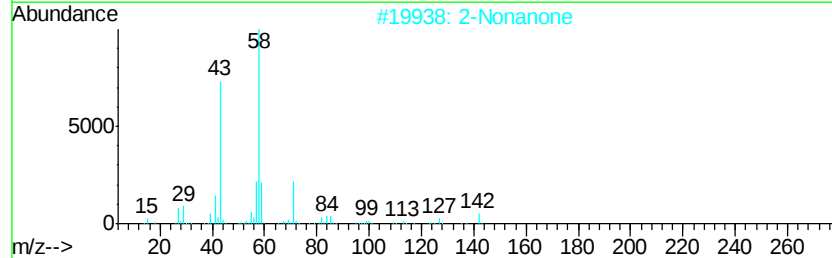
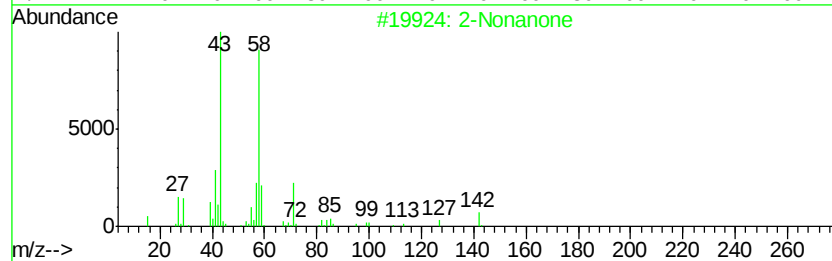
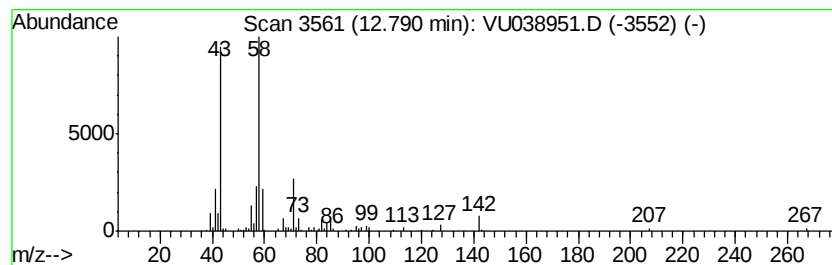
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2-Nonanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.79	0.69 ug/L	112998	1,4-Dichlorobenzene-d4	11.82

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone		142	C9H18O	000821-55-6	94
2	2-Nonanone		142	C9H18O	000821-55-6	93
3	2-Nonanone		142	C9H18O	000821-55-6	90
4	2-Dodecanone		184	C12H24O	006175-49-1	78
5	2-Dodecanone		184	C12H24O	006175-49-1	72



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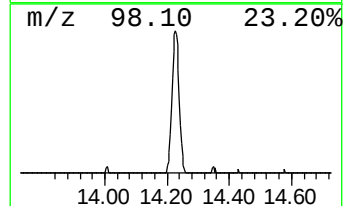
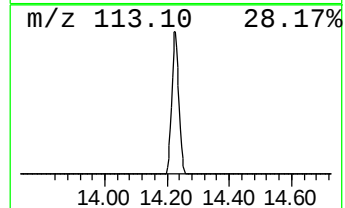
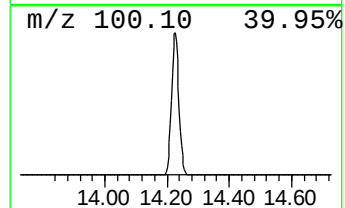
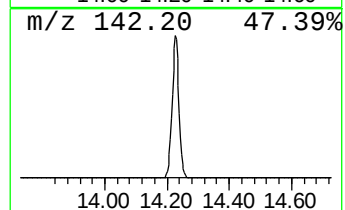
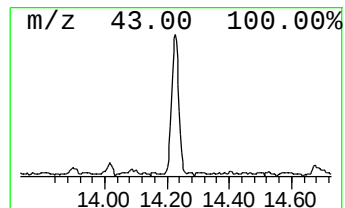
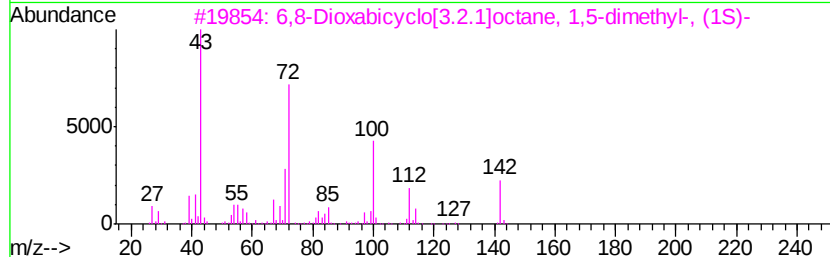
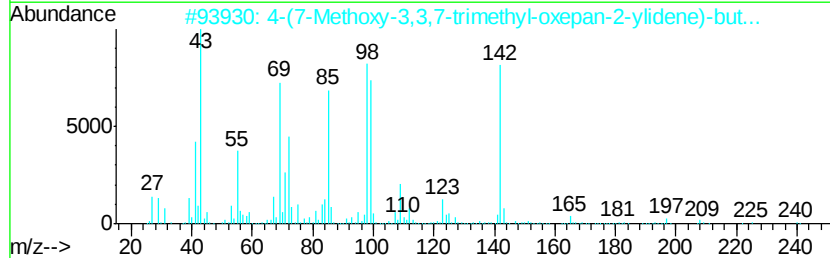
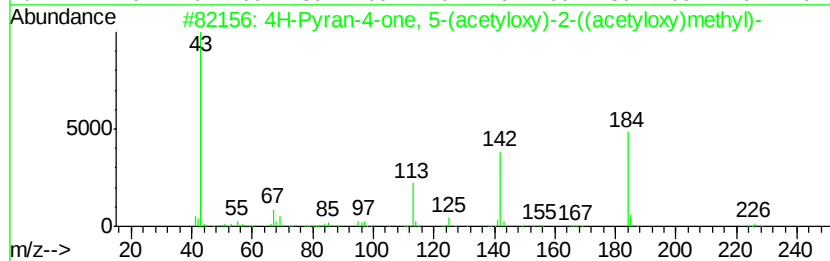
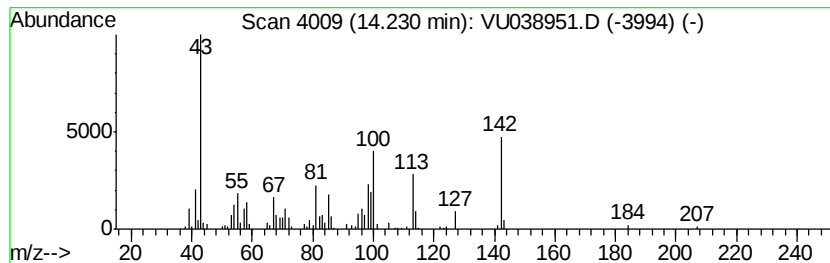
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	0.85 ug/L	138639	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	35
2		4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	35
3		6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	32
4		2-Tridecenoic acid, (E)-	212	C13H24O2	032466-55-0	27
5		1-Methylpiperidine-3-carboxylic ...	171	C9H17NO2	005166-67-6	12



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038951.D
Acq On : 17 Jun 2020 18:02
Operator : SY/MD
Sample : L3040-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

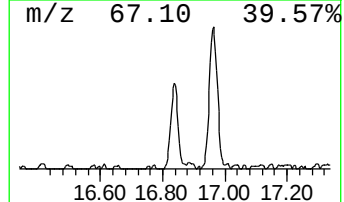
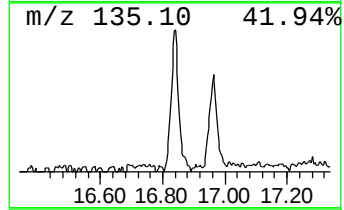
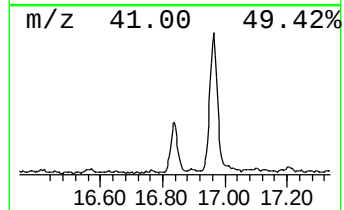
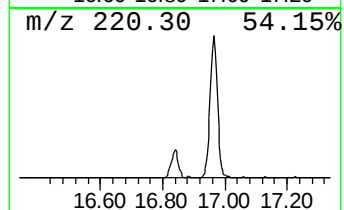
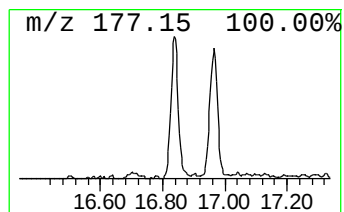
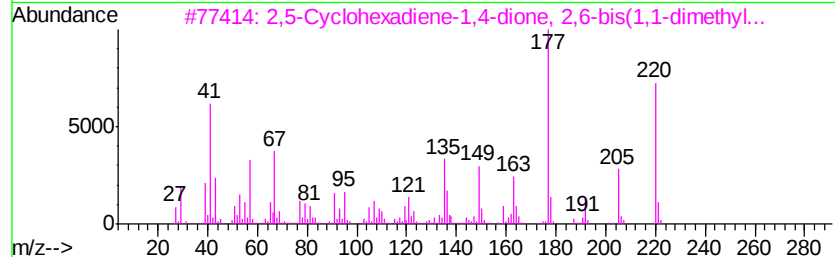
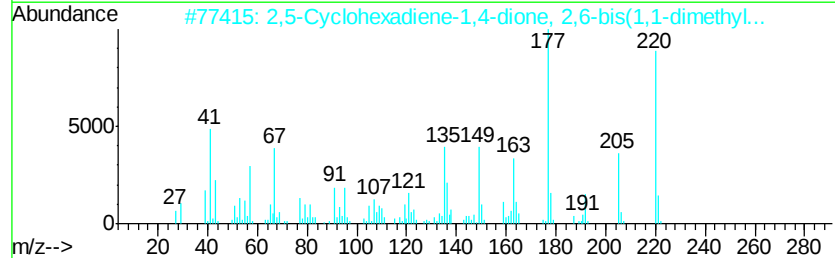
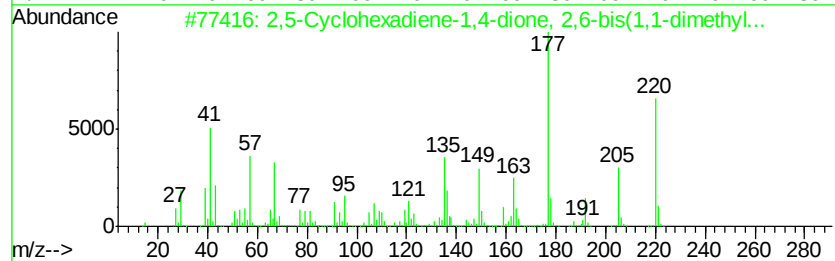
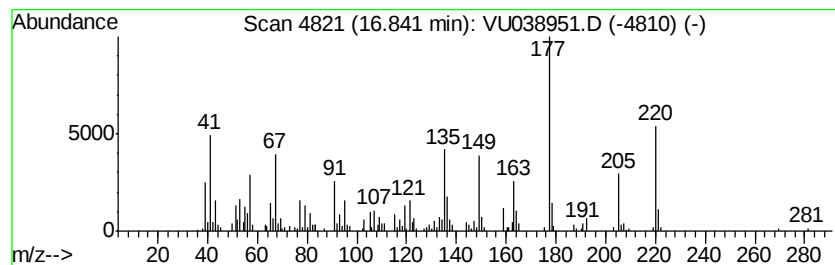
Instrument :
MSVOA_U
ClientSampleId :
F9L17

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 7 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.84	0.98 ug/L	160339	1,4-Dichlorobenzene-d4	11.82		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95	
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94	
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94	
4	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	49	
5	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	46	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU061720\
Data File : VU038951.D
Acq On : 17 Jun 2020 18:02
Operator : SY/MD
Sample : L3040-07
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L17

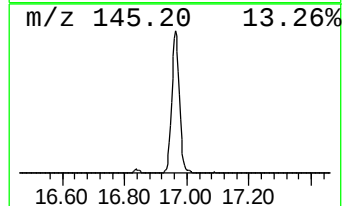
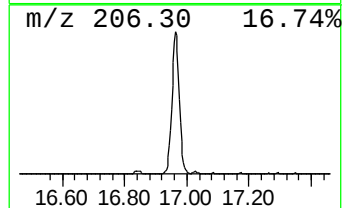
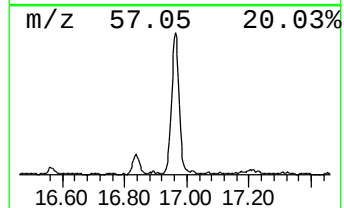
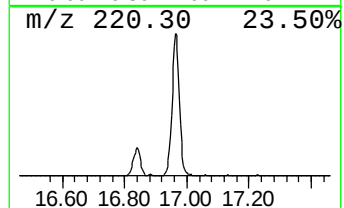
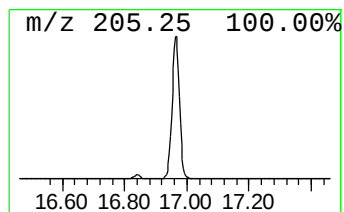
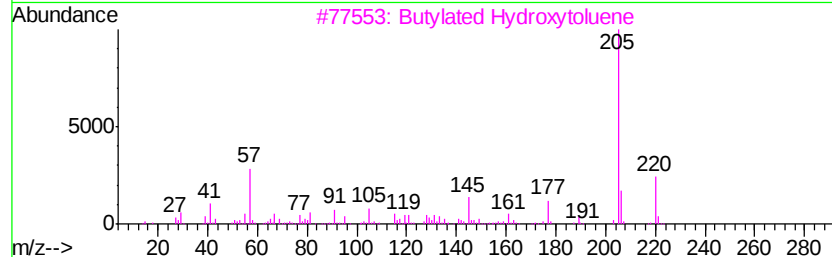
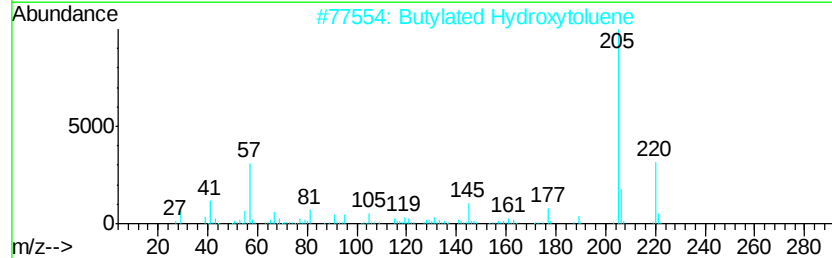
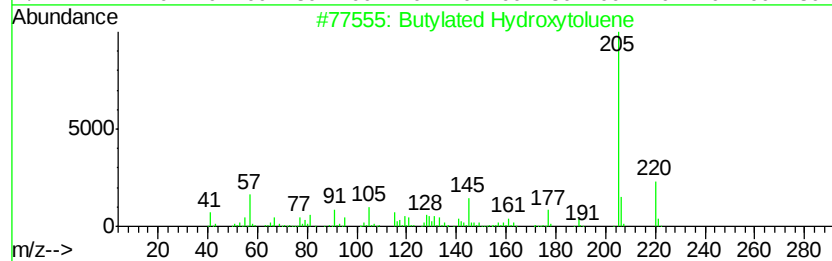
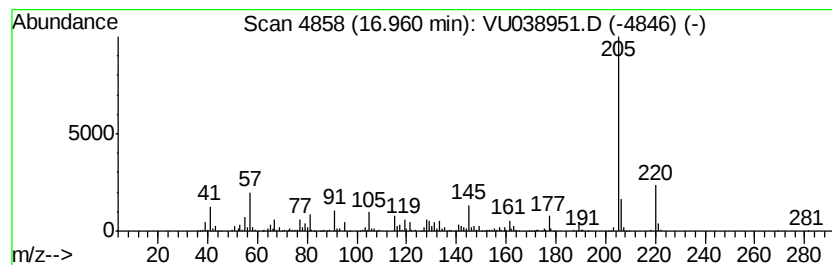
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	4.70 ug/L	768235	1,4-Dichlorobenzene-d4	11.82

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	97
3	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	97
4	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 2,4,6-tris(1-methylethyl)-		220	C15H24O	002934-07-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038951.D
Acq On : 17 Jun 2020 18:02
Operator : SY/MD
Sample : L3040-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L17

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
2-Butanone, 3,3-d...	7.23	0.6	ug/L	75721	1	6.32	625358	5.0
2-Heptanone	10.26	0.6	ug/L	93075	2	9.44	799583	5.0
1-Hexanol, 2-ethyl-	12.08	16.1	ug/L	2636260	3	11.82	817306	5.0
2-Nonanone	12.79	0.7	ug/L	112998	3	11.82	817306	5.0
unknown-01	14.23	0.8	ug/L	138639	3	11.82	817306	5.0
2,5-Cyclohexadien...	16.84	1.0	ug/L	160339	3	11.82	817306	5.0
Butylated Hydroxy...	16.96	4.7	ug/L	768235	3	11.82	817306	5.0