

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
 Data File : VU038945.D
 Acq On : 17 Jun 2020 15:44
 Operator : SY/MD
 Sample : L3040-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9L08

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	1.626	79	89	103	rVB2	125432	168048	12.01%	1.495%
2	1.941	179	187	199	rBV	155654	199107	14.23%	1.772%
3	2.604	383	393	404	rBV	276500	435549	31.13%	3.876%
4	3.099	542	547	559	rVB4	12905	19580	1.40%	0.174%
5	4.546	978	997	1013	rVB7	13714	42147	3.01%	0.375%
6	4.796	1045	1075	1111	rBV2	105200	484384	34.62%	4.310%
7	5.134	1163	1180	1200	rBV	197294	432721	30.93%	3.851%
8	5.784	1361	1382	1401	rBV2	440525	1015422	72.58%	9.036%
9	6.298	1529	1542	1561	rVB	438179	807655	57.73%	7.187%
10	6.742	1665	1680	1696	rBV	242419	465841	33.30%	4.145%
11	6.877	1709	1722	1733	rBV2	21860	40813	2.92%	0.363%
12	7.224	1804	1830	1849	rBV	97206	208104	14.87%	1.852%
13	7.603	1935	1948	1962	rBV	127092	222147	15.88%	1.977%
14	7.931	2029	2050	2065	rVB	467929	802469	57.36%	7.141%
15	8.211	2125	2137	2148	rBV2	87288	143779	10.28%	1.279%
16	8.497	2214	2226	2231	rBV2	25552	47486	3.39%	0.423%
17	8.578	2244	2251	2264	rVB8	9645	16345	1.17%	0.145%
18	8.674	2266	2281	2299	rBV	766227	1399063	100.00%	12.450%
19	9.439	2506	2519	2540	rBV	620483	1020301	72.93%	9.079%
20	9.632	2568	2579	2583	rBV4	9723	14915	1.07%	0.133%
21	9.790	2615	2628	2638	rBV3	10667	19657	1.41%	0.175%
22	9.941	2665	2675	2684	rBV3	17855	28107	2.01%	0.250%
23	10.700	2905	2911	2922	rVB4	11961	18240	1.30%	0.162%
24	10.774	2922	2934	2949	rBV	216852	346843	24.79%	3.086%
25	10.902	2959	2974	2986	rBV2	33028	56008	4.00%	0.498%
26	10.979	2987	2998	3012	rBV	16833	27749	1.98%	0.247%
27	11.825	3248	3261	3275	rBV	664321	1026385	73.36%	9.133%
28	12.082	3327	3341	3346	rBV4	13420	24357	1.74%	0.217%
29	12.204	3366	3379	3395	rVB	513237	806430	57.64%	7.176%
30	12.336	3403	3420	3433	rBV	21118	39835	2.85%	0.354%
31	12.796	3553	3563	3572	rBV3	17469	29328	2.10%	0.261%
32	12.909	3588	3598	3610	rVV4	16341	25646	1.83%	0.228%
33	13.163	3665	3677	3686	rVB4	8016	14950	1.07%	0.133%
34	14.230	3997	4009	4024	rBV2	140720	224453	16.04%	1.997%

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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	14.352	4037	4047	4061	rBV3	46471	74019	5.29%	0.659%
36	15.047	4252	4263	4272	rBV7	10849	20574	1.47%	0.183%
37	15.745	4471	4480	4492	rBV6	24477	40757	2.91%	0.363%
38	16.195	4609	4620	4630	rBV3	33944	56863	4.06%	0.506%
39	16.841	4811	4821	4830	rBV4	53460	82409	5.89%	0.733%
40	16.963	4848	4859	4874	rBV	167646	289230	20.67%	2.574%

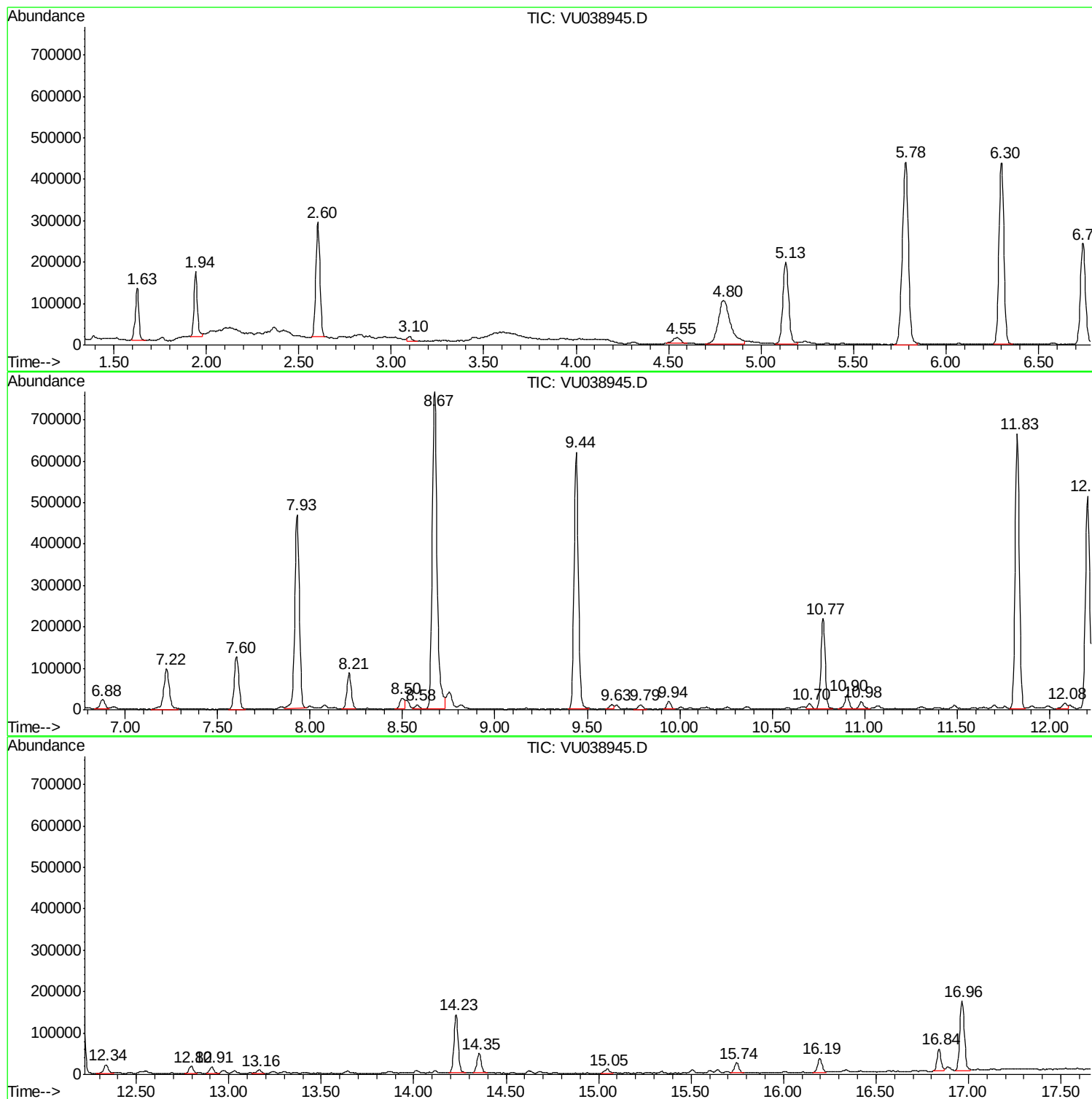
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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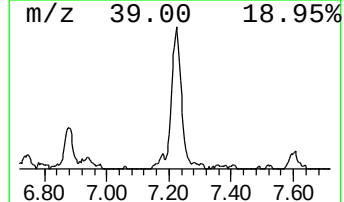
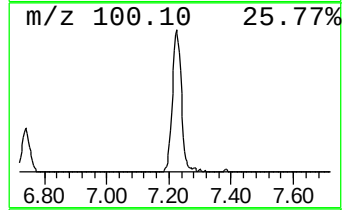
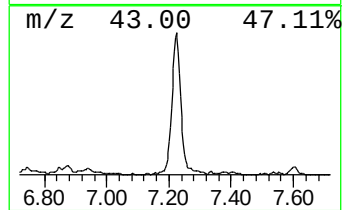
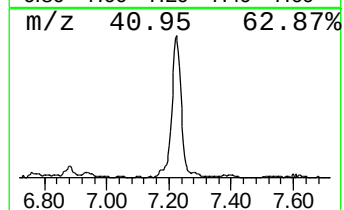
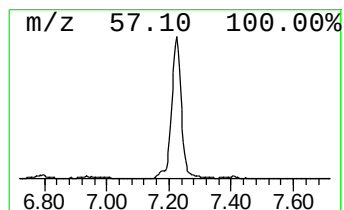
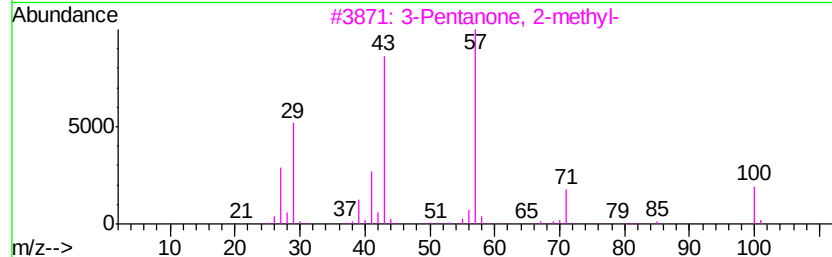
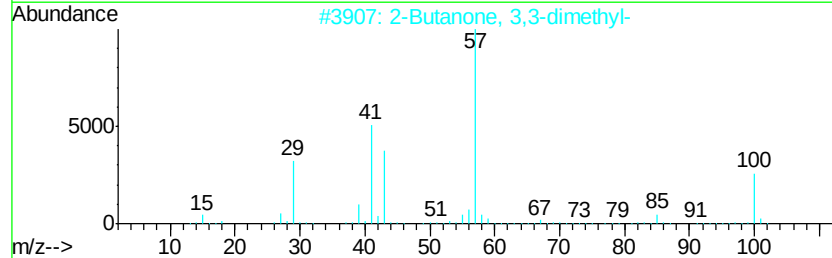
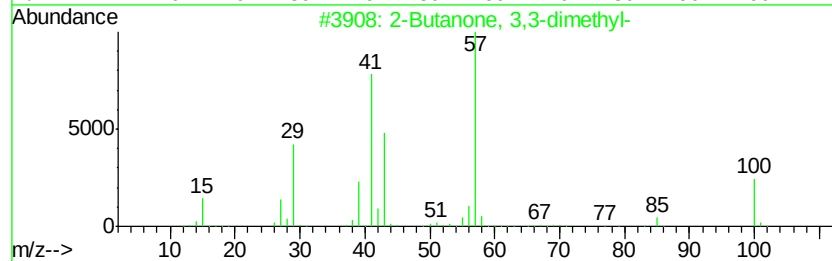
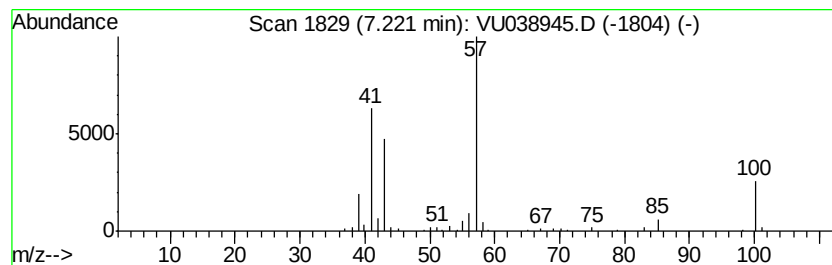
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.22	1.29 ug/L	208104	1,4-Difluorobenzene	6.30

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	90
3			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
4			3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
5			2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64



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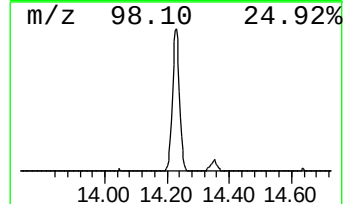
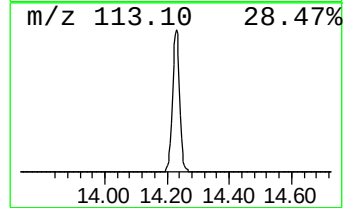
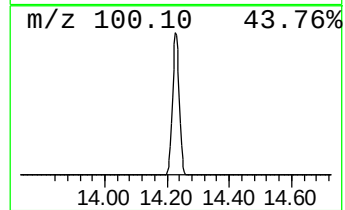
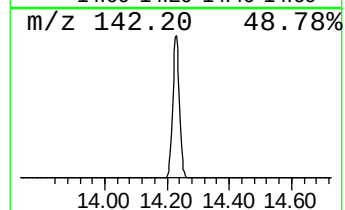
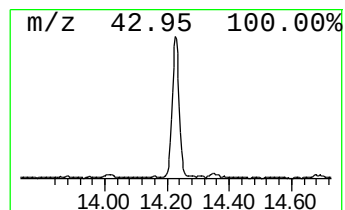
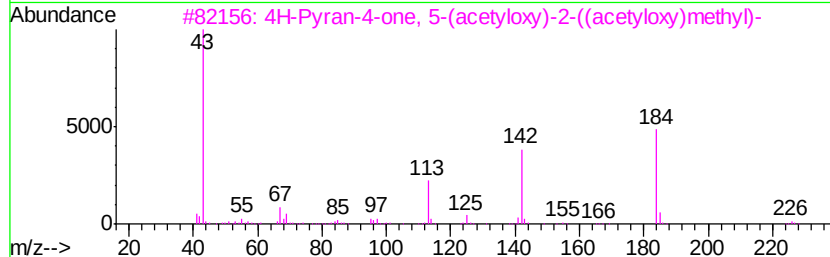
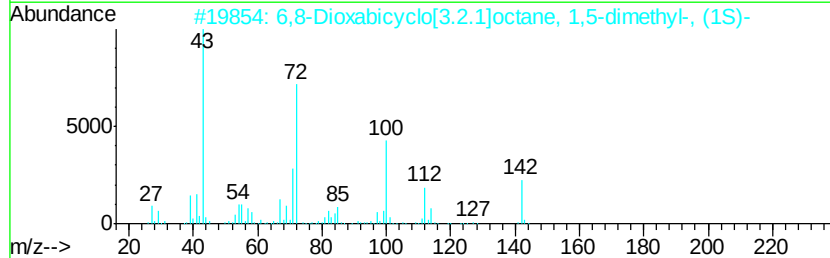
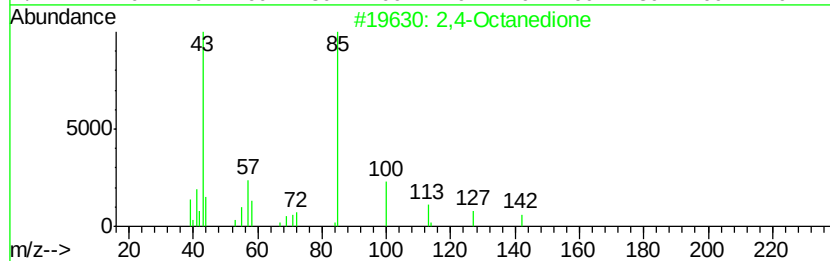
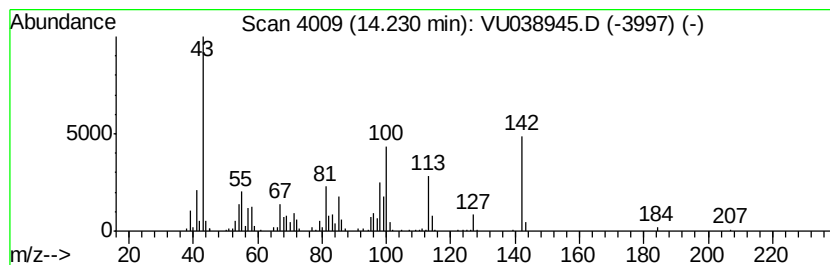
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	1.09 ug/L	224453	1,4-Dichlorobenzene-d4	11.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	32
2			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	27
3			4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	25
4			4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	25
5			Isoxazole, 3,5-dimethyl-4-nitro-	142	C5H6N2O3	001123-49-5	12



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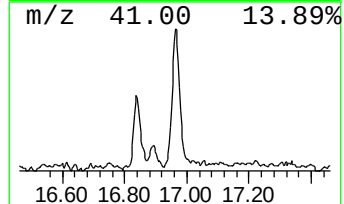
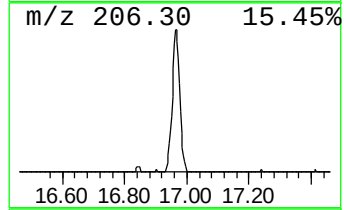
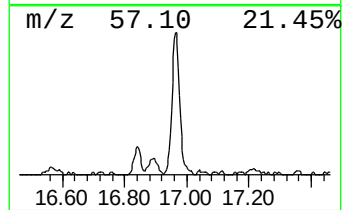
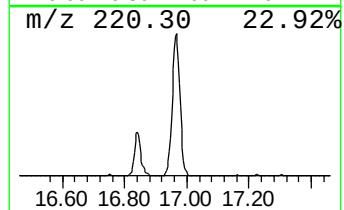
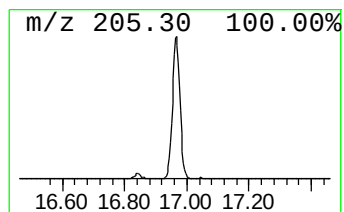
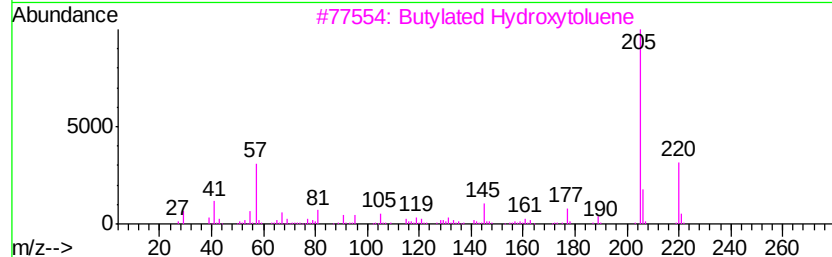
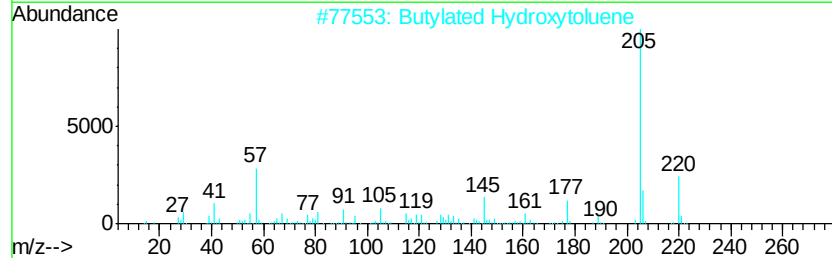
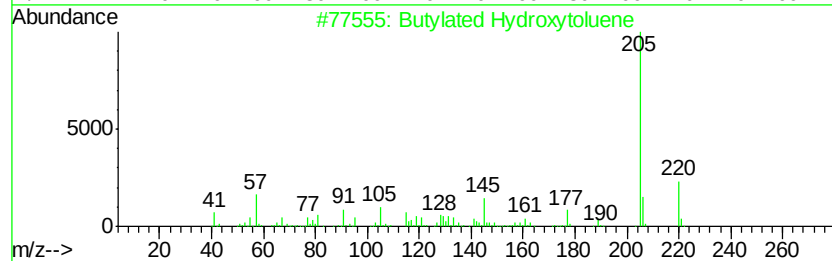
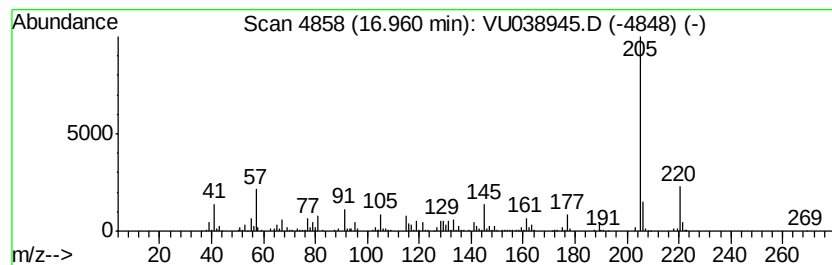
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.96	1.41 ug/L	289230	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	95
4	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 4,6-di(1,1-dimethylethyl...		220	C15H24O	000616-55-7	93



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Operator : SY/MD
Sample : L3040-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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-Butanone, 3,3-d...	7.22	1.3	ug/L	208104	1	6.30	807655	5.0
unknown-01	14.23	1.1	ug/L	224453	3	11.83	1026390	5.0
Butylated Hydroxy...	16.96	1.4	ug/L	289230	3	11.83	1026390	5.0