

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061720\
 Data File : VU038949.D
 Acq On : 17 Jun 2020 17:16
 Operator : SY/MD
 Sample : L3040-05
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9L15

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	1.617	76	86	97	rBV	127101	154879	12.46%	1.269%
2	1.755	124	129	136	rVB3	12677	16769	1.35%	0.137%
3	1.941	180	187	206	rVB	121608	168616	13.56%	1.382%
4	2.096	229	235	236	rBV	21516	20112	1.62%	0.165%
5	2.594	380	390	408	rBV	276045	446119	35.88%	3.655%
6	2.819	453	460	474	rVB3	17939	39148	3.15%	0.321%
7	4.485	964	978	994	rBV5	21533	63945	5.14%	0.524%
8	4.777	1043	1069	1113	rBV2	98575	447332	35.98%	3.665%
9	5.131	1159	1179	1206	rVB	207804	486749	39.15%	3.988%
10	5.787	1362	1383	1411	rBV2	430948	1026816	82.59%	8.413%
11	6.305	1531	1544	1563	rVB	359240	639741	51.46%	5.242%
12	6.745	1667	1681	1700	rBV2	253541	495103	39.82%	4.057%
13	7.224	1817	1830	1843	rVB3	32862	63572	5.11%	0.521%
14	7.603	1936	1948	1965	rBV	126275	218559	17.58%	1.791%
15	7.935	2037	2051	2064	rVB	445992	759625	61.10%	6.224%
16	8.079	2088	2096	2105	rVB2	10424	16463	1.32%	0.135%
17	8.211	2122	2137	2153	rVB	81353	138125	11.11%	1.132%
18	8.523	2216	2234	2244	rBV6	8255	21649	1.74%	0.177%
19	8.584	2244	2253	2264	rBV7	11876	20502	1.65%	0.168%
20	8.671	2265	2280	2291	rBV	704929	1243282	100.00%	10.187%
21	8.726	2292	2297	2312	rVB3	131227	238995	19.22%	1.958%
22	9.439	2507	2519	2544	rBV	493272	825191	66.37%	6.761%
23	9.661	2581	2588	2597	rVB2	19396	29649	2.38%	0.243%
24	9.790	2613	2628	2640	rBV6	13297	30458	2.45%	0.250%
25	9.941	2663	2675	2687	rBV	40761	66195	5.32%	0.542%
26	10.150	2723	2740	2754	rBV5	16275	36702	2.95%	0.301%
27	10.253	2756	2772	2787	rBV	72360	126095	10.14%	1.033%
28	10.362	2798	2806	2824	rVB6	12501	24308	1.96%	0.199%
29	10.700	2903	2911	2922	rVB2	26890	41146	3.31%	0.337%
30	10.774	2922	2934	2958	rVB	213159	351170	28.25%	2.877%
31	10.906	2969	2975	2984	rVB10	8520	13612	1.09%	0.112%
32	10.980	2984	2998	3013	rBV	41332	71574	5.76%	0.586%
33	11.066	3016	3025	3036	rVB6	13293	22483	1.81%	0.184%
34	11.481	3145	3154	3164	rBV4	24079	35147	2.83%	0.288%

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 ALS Vial : 1 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
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 Title : TRACE VOA SOM01.0

35	11.584	3177	3186	3197	rBV3	36274	56364	4.53%	0.462%
36	11.697	3215	3221	3231	rVV4	10951	16832	1.35%	0.138%
37	11.825	3248	3261	3275	rVB	527044	836573	67.29%	6.854%
38	11.899	3275	3284	3294	rBV6	7328	13999	1.13%	0.115%
39	11.989	3306	3312	3321	rVB5	8494	13825	1.11%	0.113%
40	12.076	3326	3339	3366	rBV	172751	399105	32.10%	3.270%
41	12.205	3368	3379	3396	rVB	517406	842609	67.77%	6.904%
42	12.336	3411	3420	3425	rBV	17760	28489	2.29%	0.233%
43	12.372	3426	3431	3446	rVB3	25193	40050	3.22%	0.328%
44	12.793	3553	3562	3576	rBV	48999	77585	6.24%	0.636%
45	12.906	3588	3597	3610	rVB6	19490	30505	2.45%	0.250%
46	12.970	3610	3617	3627	rVV9	8021	12562	1.01%	0.103%
47	13.024	3627	3634	3643	rVB5	8829	12817	1.03%	0.105%
48	13.163	3669	3677	3686	rVB3	8886	15695	1.26%	0.129%
49	13.423	3746	3758	3767	rBV3	6605	14812	1.19%	0.121%
50	13.639	3817	3825	3833	rVB3	19515	27424	2.21%	0.225%
51	14.015	3933	3942	3949	rBV7	12510	19733	1.59%	0.162%
52	14.089	3956	3965	3976	rBV7	9399	19675	1.58%	0.161%
53	14.227	3998	4008	4022	rVB2	88640	141918	11.41%	1.163%
54	14.684	4141	4150	4164	rBV8	14355	30956	2.49%	0.254%
55	14.873	4201	4209	4215	rBV4	10428	17637	1.42%	0.145%
56	15.047	4255	4263	4273	rVB6	7908	12625	1.02%	0.103%
57	15.745	4470	4480	4495	rVB8	26789	50318	4.05%	0.412%
58	16.192	4608	4619	4632	rBV4	25046	44057	3.54%	0.361%
59	16.413	4682	4688	4697	rVB10	8266	13220	1.06%	0.108%
60	16.838	4810	4820	4836	rBV4	87280	148962	11.98%	1.221%
61	16.963	4847	4859	4874	rBV	517768	866629	69.70%	7.101%

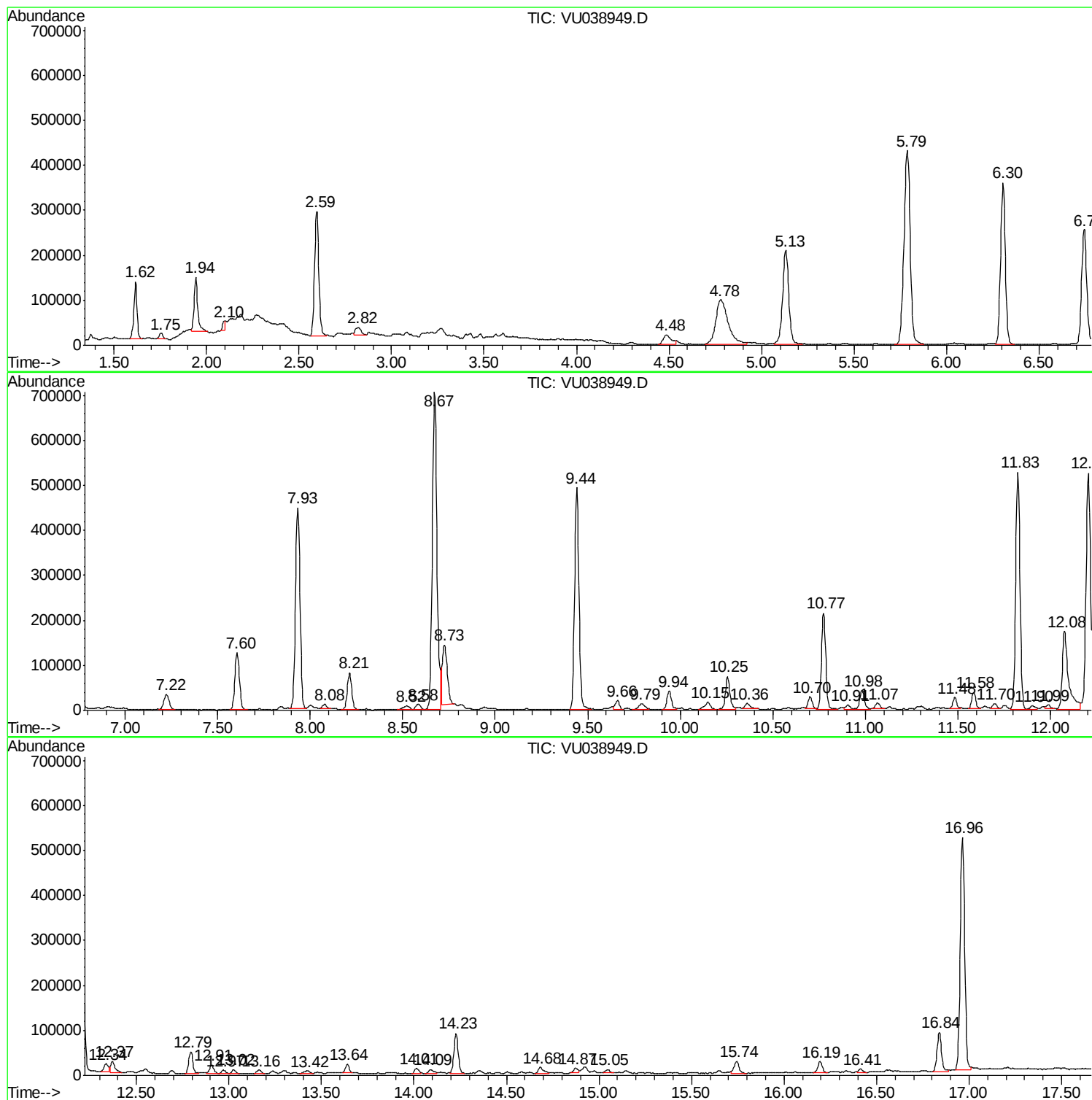
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ClientSampled :
F9L15

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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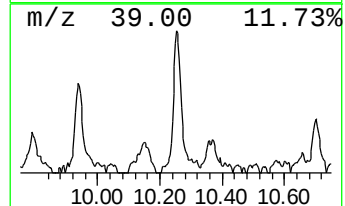
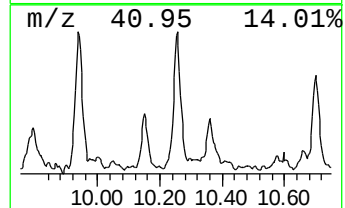
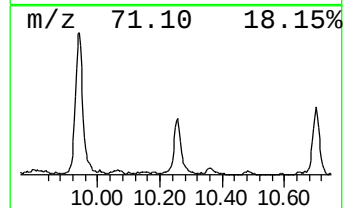
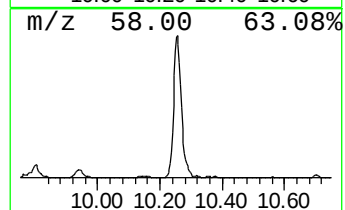
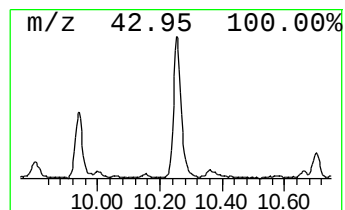
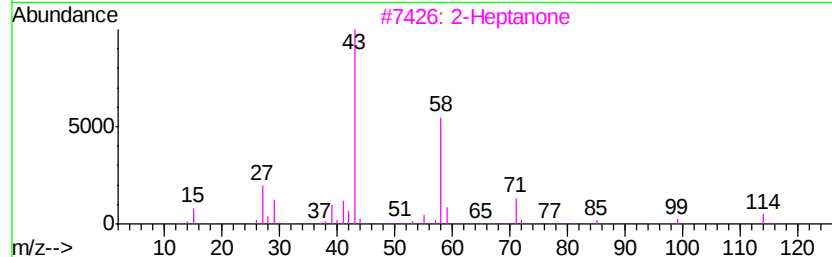
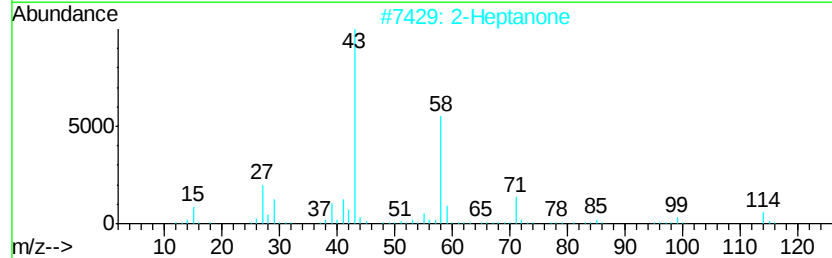
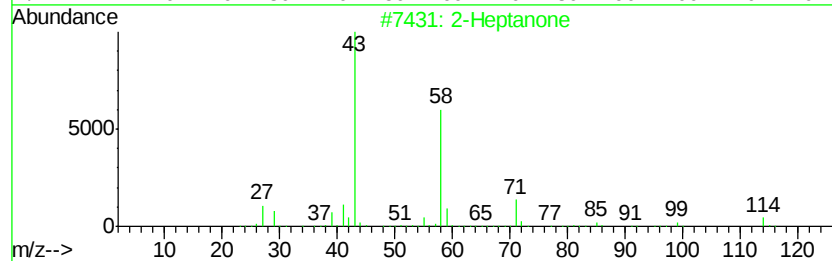
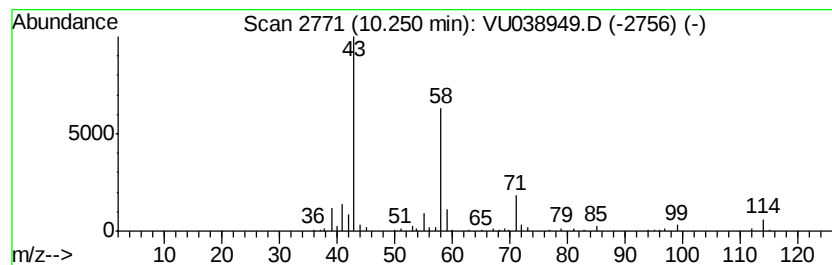
Instrument :
MSVOA_U
ClientSampleId :
F9L15

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 2 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.25	0.76 ug/L	126095	Chlorobenzene-d5	9.44		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone		114	C7H14O	000110-43-0	90
2	2-Heptanone		114	C7H14O	000110-43-0	87
3	2-Heptanone		114	C7H14O	000110-43-0	87
4	2-Heptanone		114	C7H14O	000110-43-0	72
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 :
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ClientSampleId :
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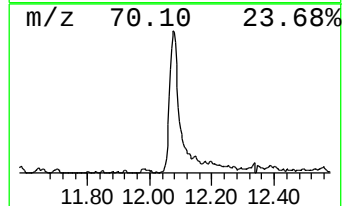
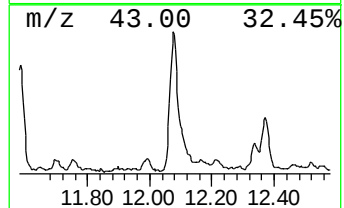
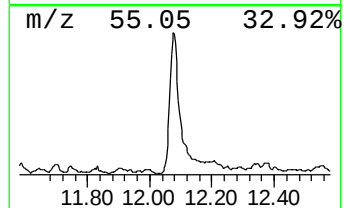
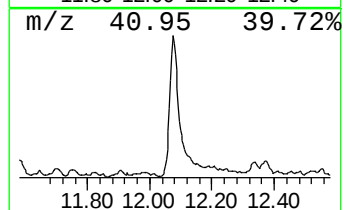
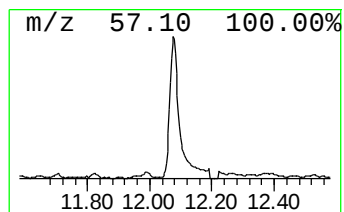
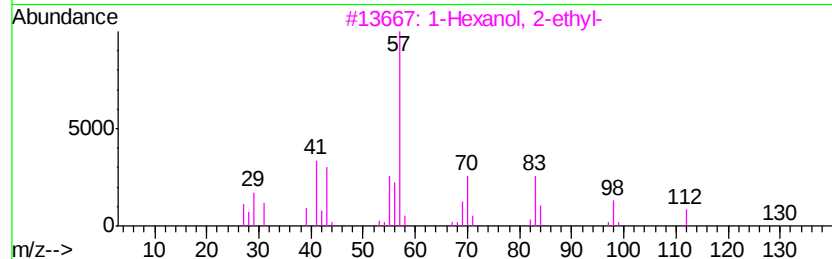
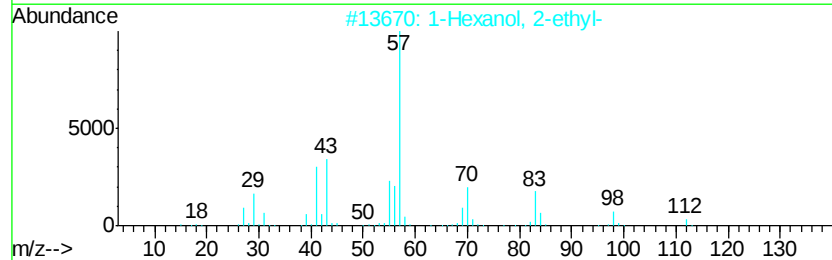
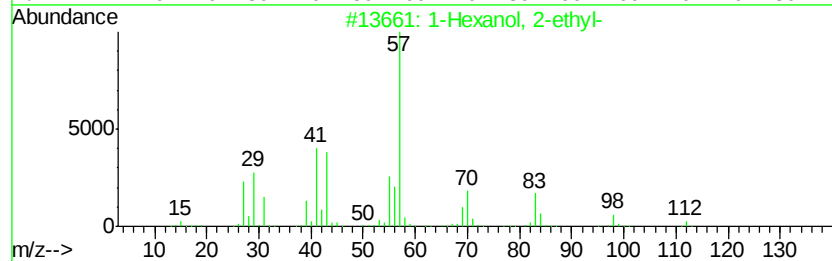
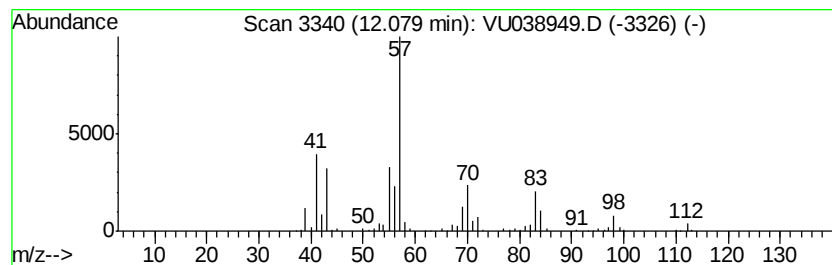
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.08	2.39 ug/L	399105	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	90
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5		Decane, 5,6-dipropyl-	226	C16H34	119209-20-0	50



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

Instrument :
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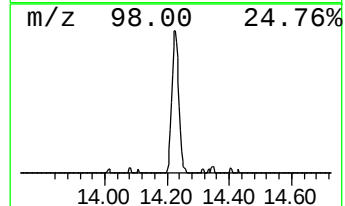
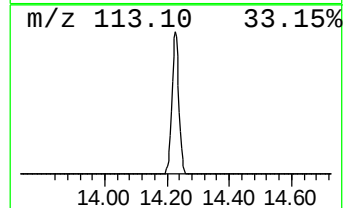
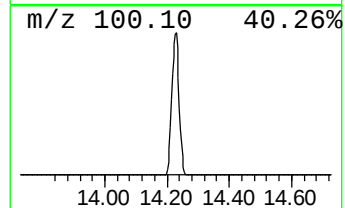
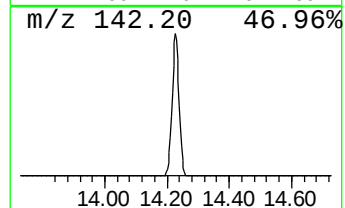
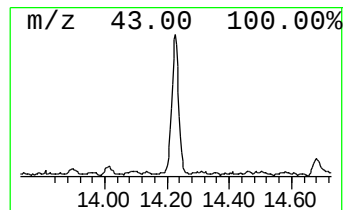
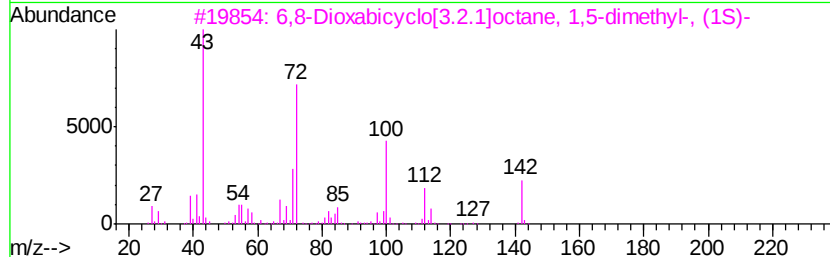
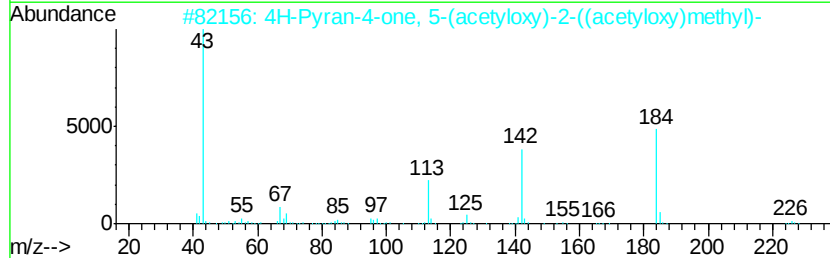
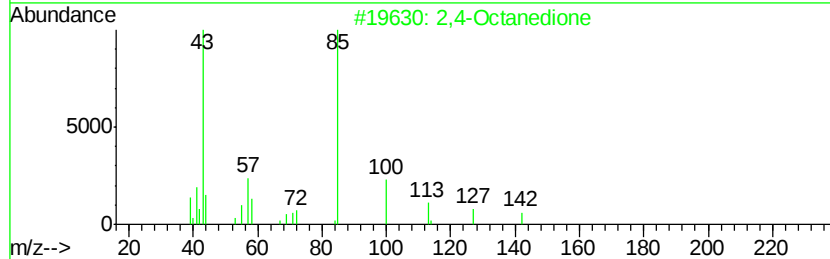
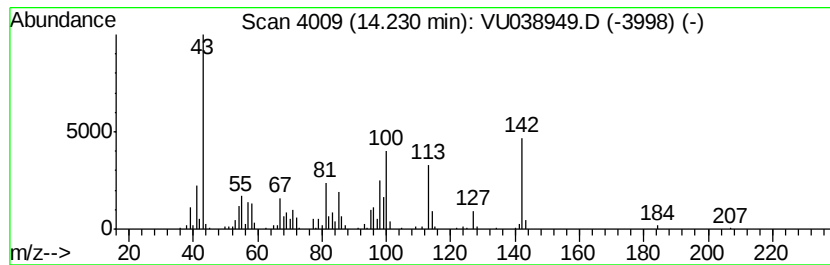
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	0.85 ug/L	141918	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4-Octanedione	142	C8H14O2	014090-87-0	43
2		4H-Pyran-4-one, 5-(acetyloxy)-2-...	226	C10H10O6	026209-93-8	25
3		6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	22
4		5-Undecanone, 2-methyl-	184	C12H24O	050639-02-6	12
5		Isoxazole, 3,5-dimethyl-4-nitro-	142	C5H6N2O3	001123-49-5	12



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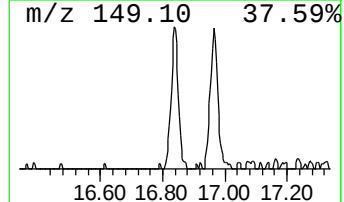
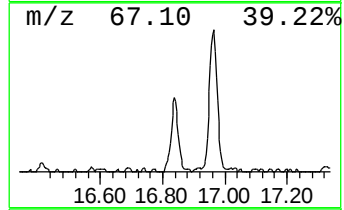
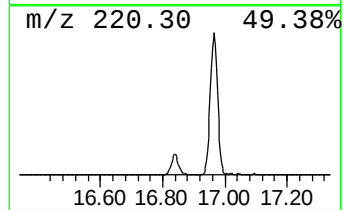
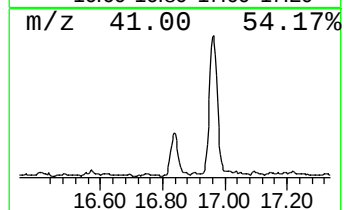
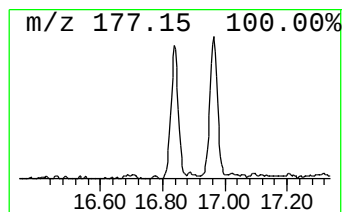
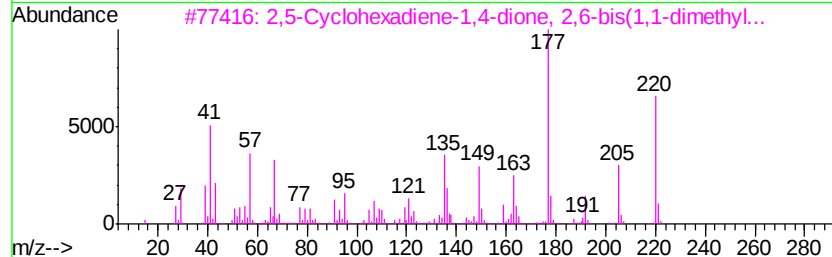
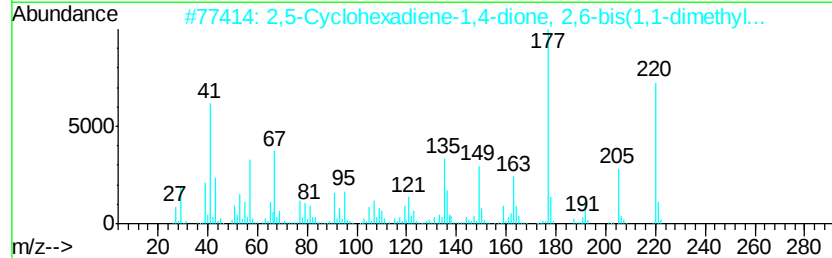
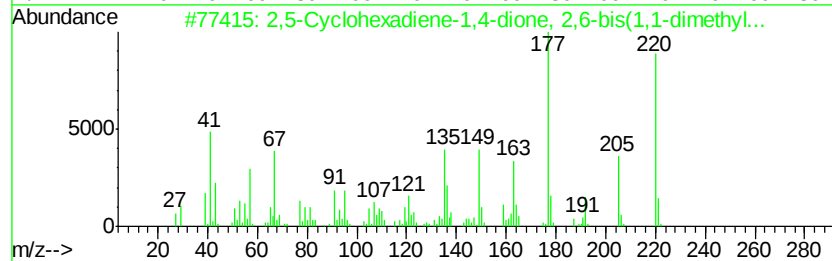
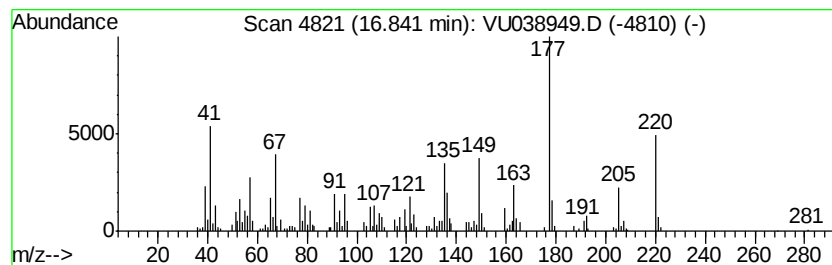
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.84	0.89 ug/L	148962	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
3		2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
4		2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	55
5		Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	53



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

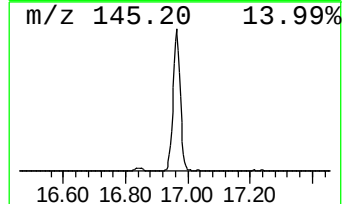
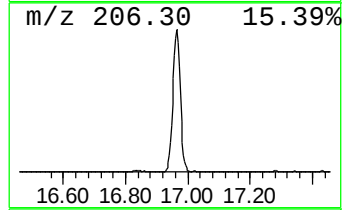
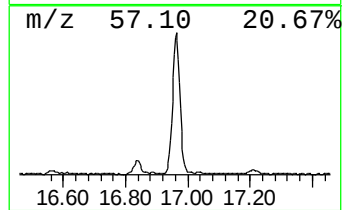
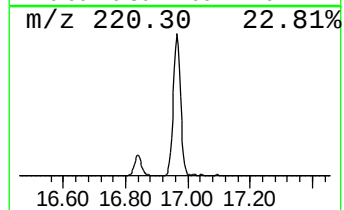
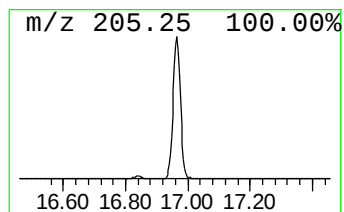
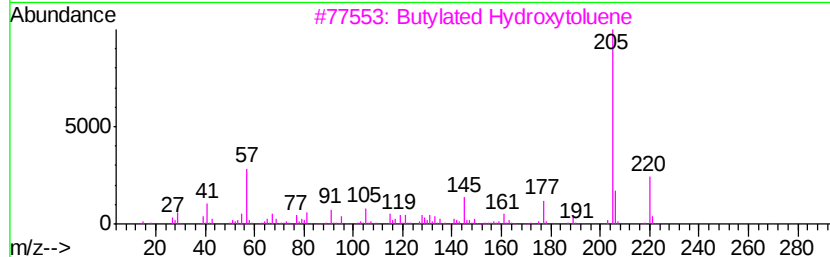
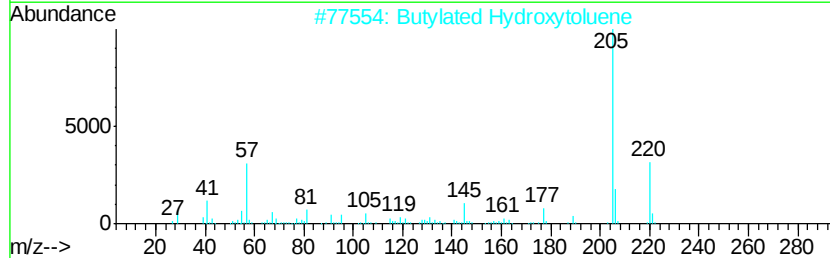
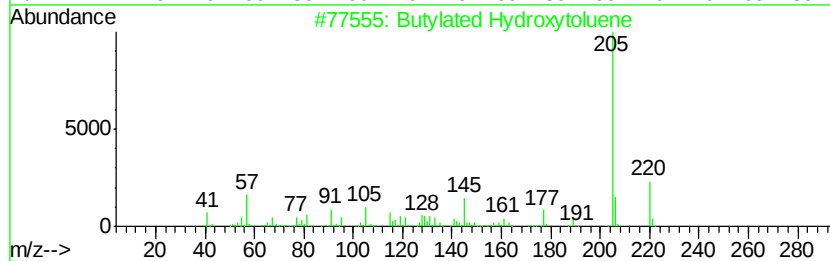
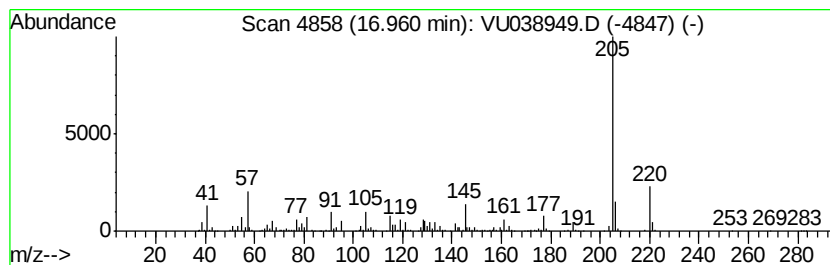
Instrument :
MSVOA_U
ClientSampleId :
F9L15

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	5.18 ug/L	866629	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	97
3	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	94
4	Butylated	Hydroxytoluene	220	C15H24O	000128-37-0	94
5	Phenol, 4,6-di(1,1-dimethylethyl...		220	C15H24O	000616-55-7	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU061720\
Data File : VU038949.D
Acq On : 17 Jun 2020 17:16
Operator : SY/MD
Sample : L3040-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9L15

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-Heptanone	10.25	0.8	ug/L	126095	2	9.44	825191	5.0
1-Hexanol, 2-ethyl-	12.08	2.4	ug/L	399105	3	11.83	836573	5.0
unknown-01	14.23	0.8	ug/L	141918	3	11.83	836573	5.0
2,5-Cyclohexadien...	16.84	0.9	ug/L	148962	3	11.83	836573	5.0
Butylated Hydroxy...	16.96	5.2	ug/L	866629	3	11.83	836573	5.0