

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
 Data File : VU042122.D
 Acq On : 20 Jan 2021 22:21
 Operator : SY/MD
 Sample : M1180-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F1E08

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\SOMUTR012021WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC: VU042122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	71	81	89	rVB	53264	65221	12.74%	1.472%
2	1.916	171	179	189	rVB	41236	51437	10.04%	1.161%
3	2.420	328	336	347	rVB7	3014	5758	1.12%	0.130%
4	2.572	371	383	398	rBV	94375	152891	29.86%	3.451%
5	4.459	956	970	981	rBV7	2134	5792	1.13%	0.131%
6	4.684	1014	1040	1091	rBV2	30951	205225	40.08%	4.633%
7	5.073	1146	1161	1184	rVB	79897	176521	34.47%	3.985%
8	5.732	1345	1366	1392	rBV2	160922	420741	82.16%	9.498%
9	6.256	1516	1529	1548	rVB	143836	272945	53.30%	6.162%
10	6.700	1653	1667	1686	rBV	100702	197337	38.54%	4.455%
11	7.179	1799	1816	1830	rBV2	14778	31362	6.12%	0.708%
12	7.575	1926	1939	1957	rBV	60527	107707	21.03%	2.431%
13	7.906	2029	2042	2058	rBV	203320	345930	67.55%	7.809%
14	7.976	2059	2064	2076	rVV5	2711	5552	1.08%	0.125%
15	8.044	2076	2085	2096	rVB3	4055	8311	1.62%	0.188%
16	8.189	2117	2130	2143	rBV	40328	67422	13.17%	1.522%
17	8.497	2216	2226	2236	rBV5	3141	5426	1.06%	0.122%
18	8.562	2236	2246	2257	rVB5	6551	10388	2.03%	0.235%
19	8.645	2257	2272	2284	rBV	272852	512092	100.00%	11.560%
20	9.423	2499	2514	2535	rBV	202776	340045	66.40%	7.676%
21	9.645	2578	2583	2593	rVB3	4607	6849	1.34%	0.155%
22	9.780	2614	2625	2634	rBV5	4000	8481	1.66%	0.191%
23	9.925	2660	2670	2682	rBV	15798	25865	5.05%	0.584%
24	10.137	2724	2736	2748	rVB5	4514	9026	1.76%	0.204%
25	10.243	2756	2769	2782	rBV	21359	36142	7.06%	0.816%
26	10.349	2795	2802	2812	rBV6	3106	5618	1.10%	0.127%
27	10.693	2900	2909	2920	rVB3	11997	18282	3.57%	0.413%
28	10.764	2920	2931	2943	rBV	81539	129173	25.22%	2.916%
29	10.973	2986	2996	3007	rBV	16996	26956	5.26%	0.609%
30	11.060	3012	3023	3032	rBV6	4585	8655	1.69%	0.195%
31	11.478	3146	3153	3163	rVB4	3722	5307	1.04%	0.120%
32	11.581	3176	3185	3195	rBV2	12635	19012	3.71%	0.429%
33	11.819	3248	3259	3277	rVB	211187	341129	66.61%	7.701%
34	12.070	3324	3337	3364	rBV	129770	249837	48.79%	5.640%
35	12.201	3367	3378	3400	rVB	201628	325097	63.48%	7.339%
36	12.330	3411	3418	3426	rBV	6235	9316	1.82%	0.210%

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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\SOMUTR012021WMA.M
Title : TRACE VOA SOM01.0

37	12.780	3548	3558	3568	rBV3	9006	13401	2.62%	0.303%
38	12.896	3585	3594	3603	rVB5	6559	9411	1.84%	0.212%
39	14.201	3989	4000	4013	rVB	31587	47592	9.29%	1.074%
40	16.143	4596	4604	4614	rBV5	4049	5124	1.00%	0.116%
41	16.899	4827	4839	4852	rBV	93443	141402	27.61%	3.192%

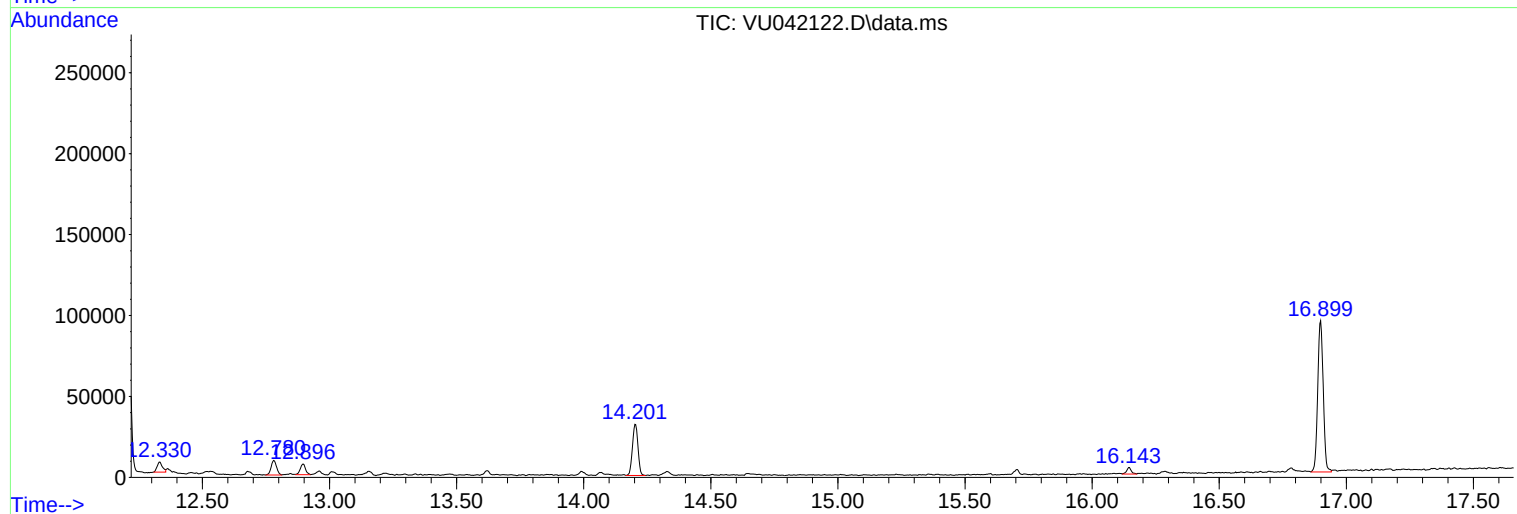
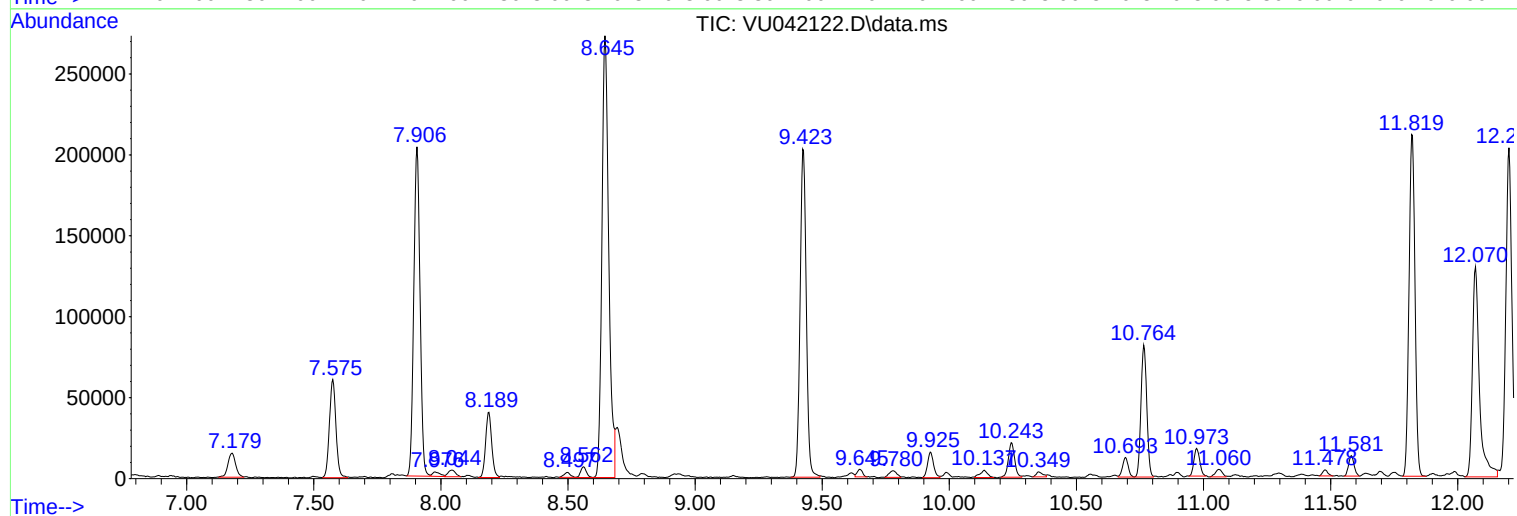
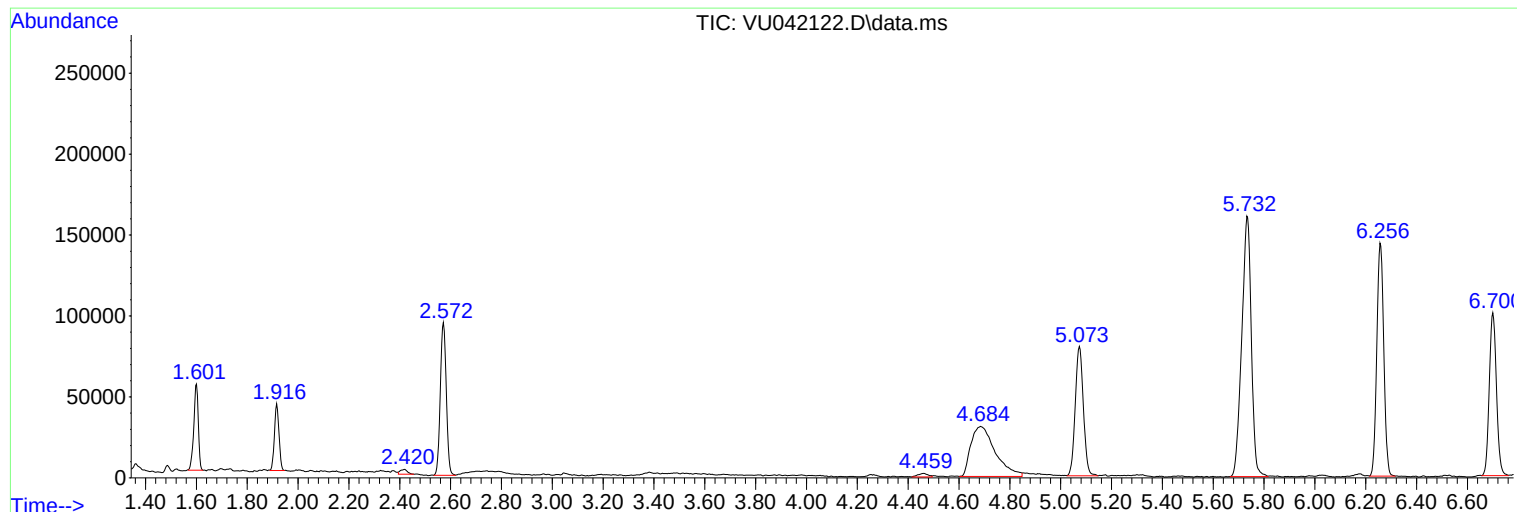
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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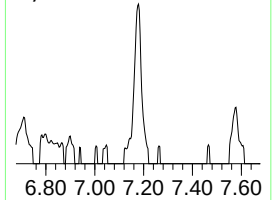
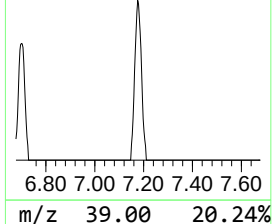
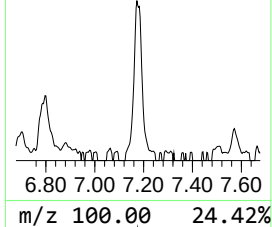
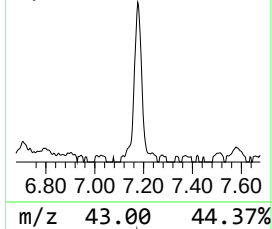
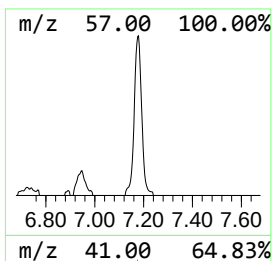
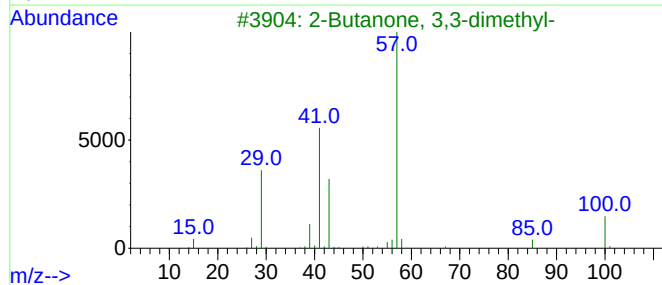
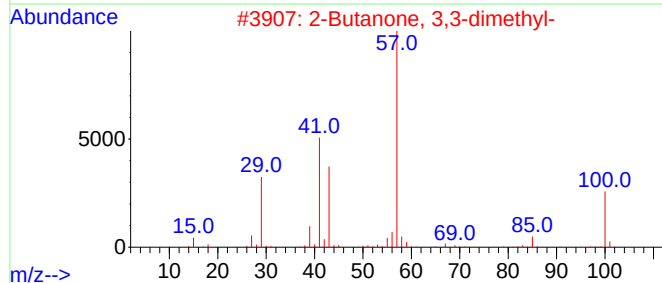
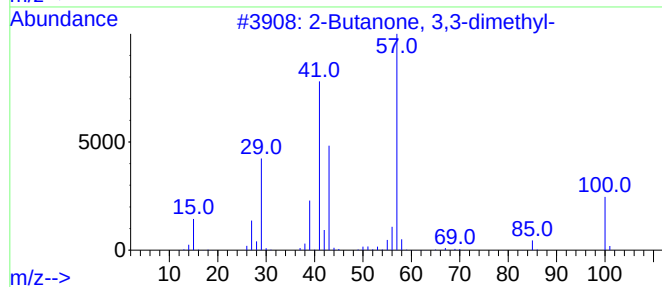
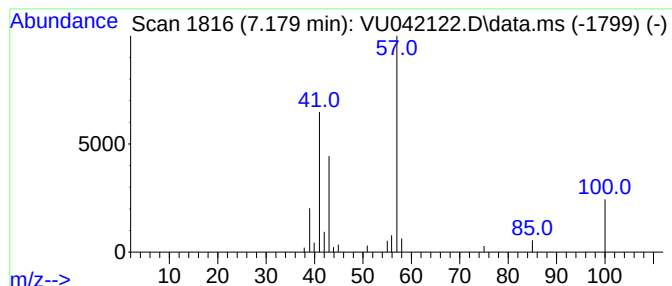
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.179	0.57 ug/L	31362	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	90
2	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	86
3	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	47
4	Diazene, bis(1,1-dimethylethyl)-			142	C8H18N2	000927-83-3	47
5	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	40



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Instrument :
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ClientSampleId :
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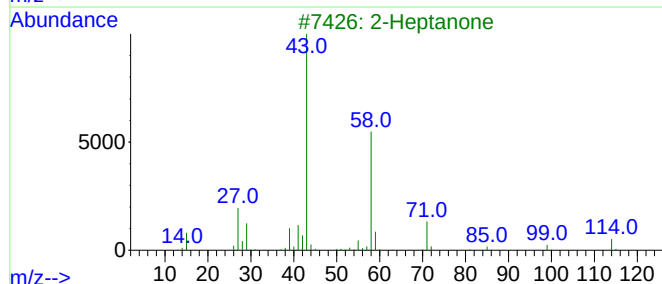
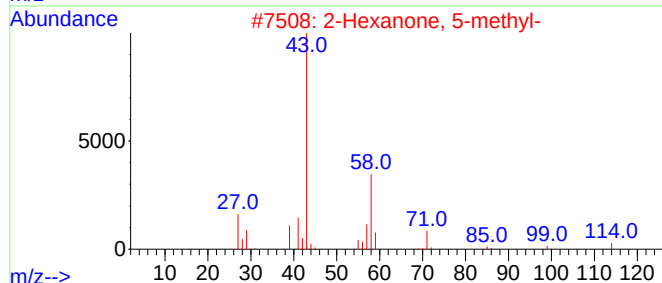
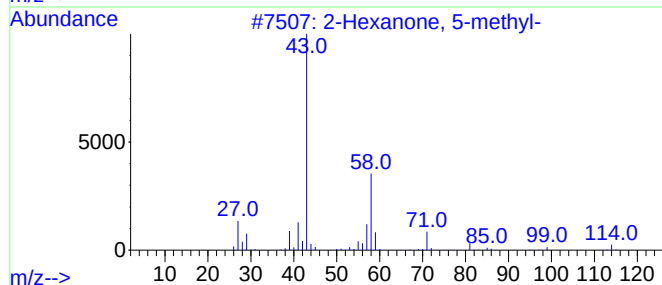
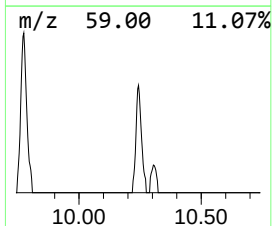
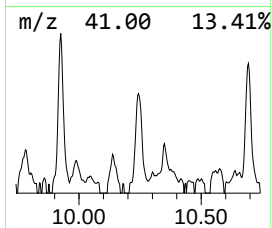
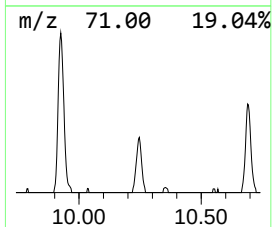
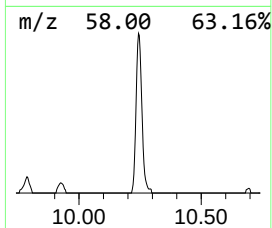
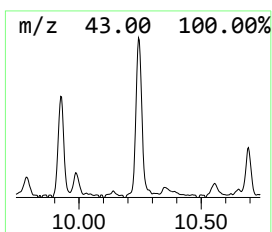
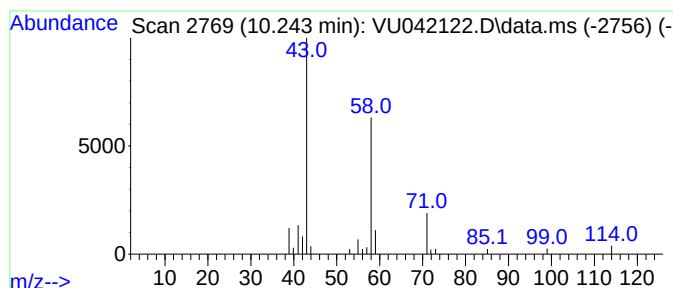
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 2-Hexanone, 5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.243	0.53 ug/L	36142	Chlorobenzene-d5	9.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90
2			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	83
3			2-Heptanone	114	C7H14O	000110-43-0	80
4			2-Heptanone	114	C7H14O	000110-43-0	80
5			2-Heptanone	114	C7H14O	000110-43-0	58



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Instrument :
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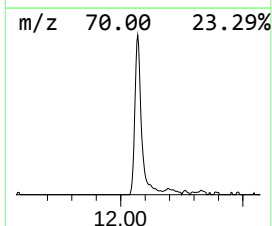
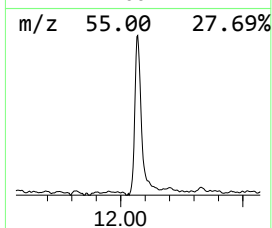
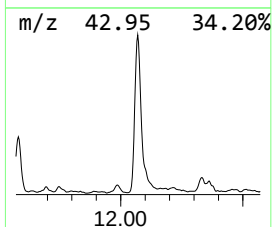
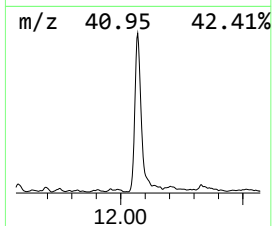
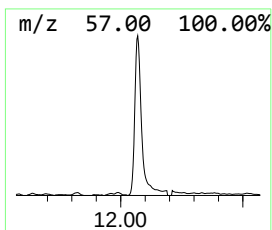
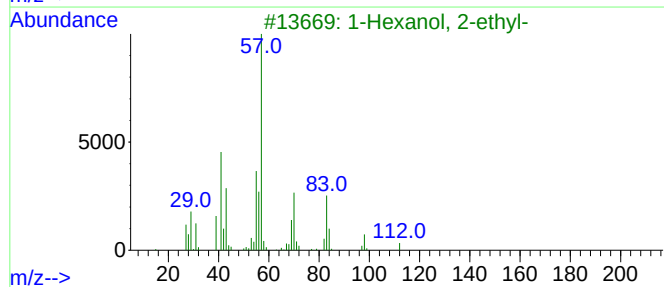
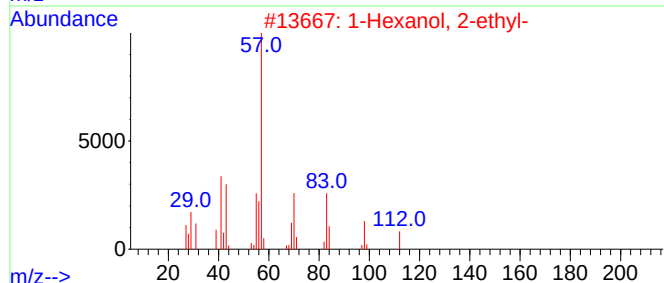
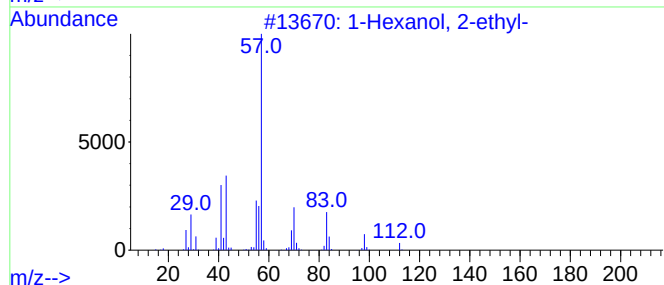
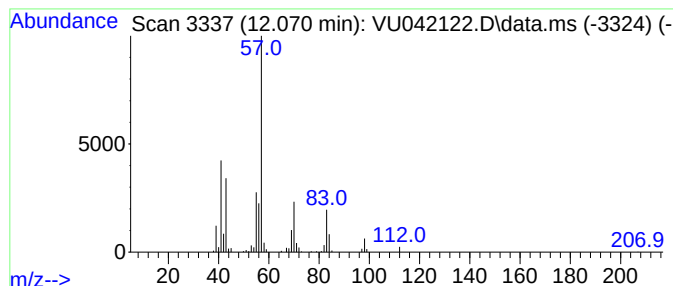
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	3.66 ug/L	249837	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	74
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56



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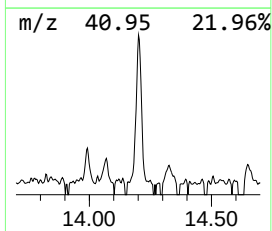
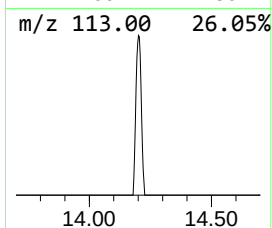
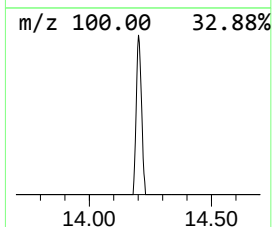
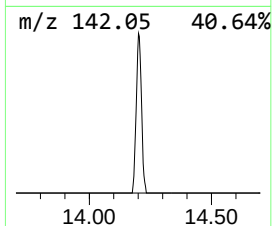
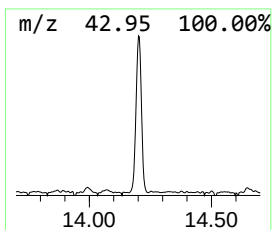
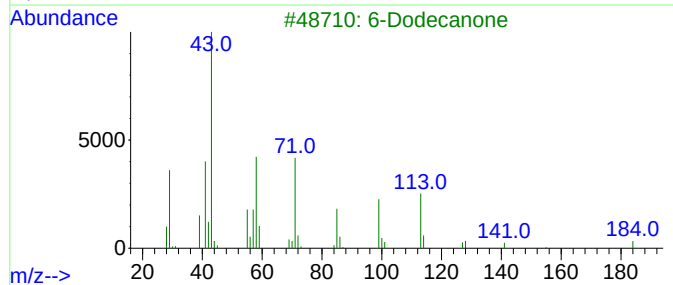
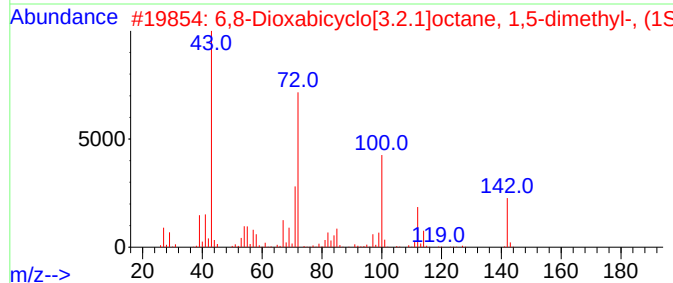
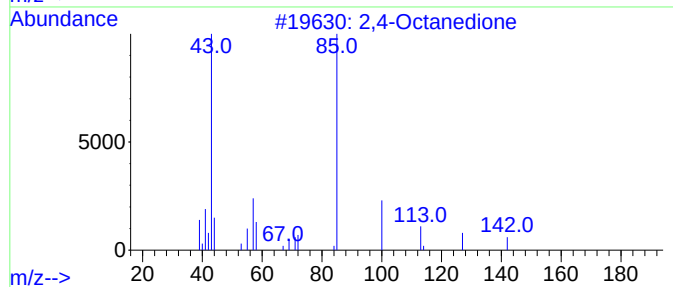
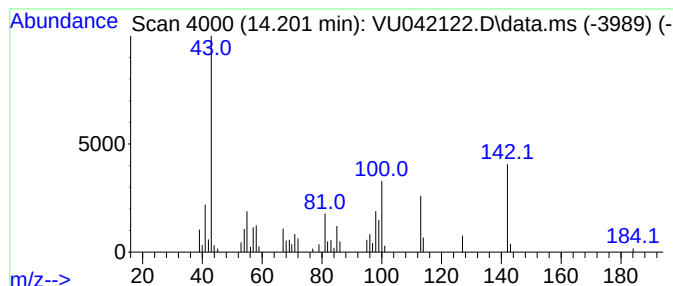
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 2,4-Octanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	0.70 ug/L	47592	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	50
2			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	32
3			6-Dodecanone	184	C12H24O	006064-27-3	16
4			6-Dodecanone	184	C12H24O	006064-27-3	14
5			2,4-Pentanedione, 3-ethyl-	128	C7H12O2	001540-34-7	10



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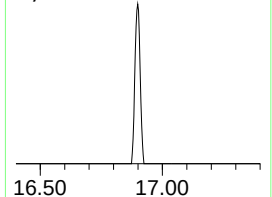
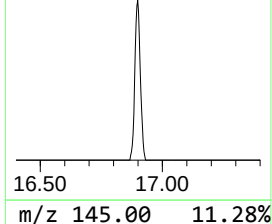
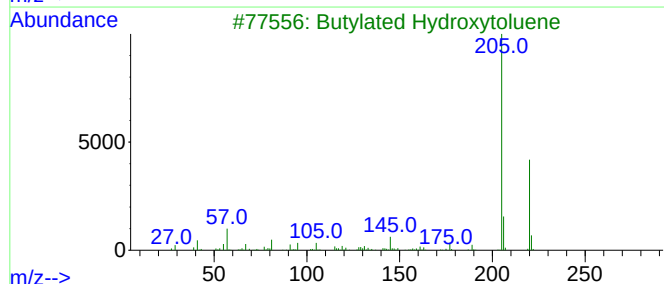
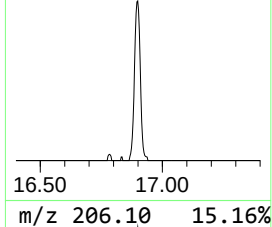
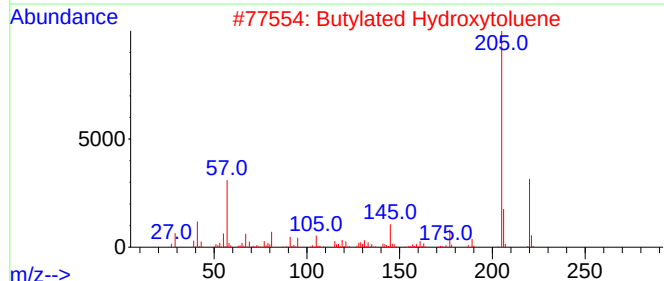
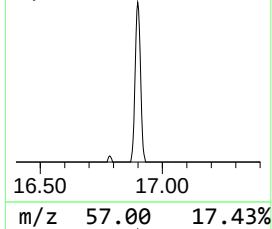
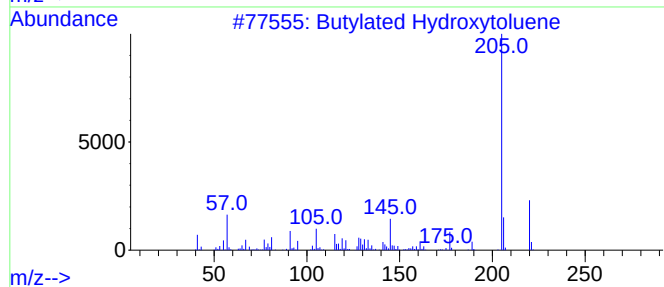
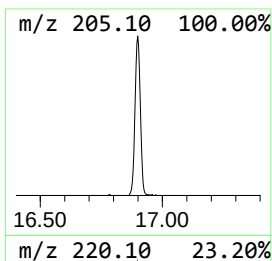
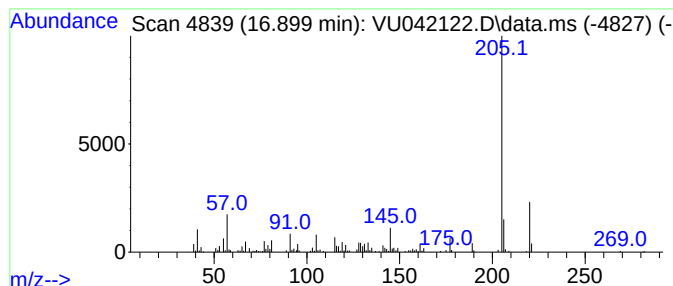
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	2.07 ug/L	141402	1,4-Dichlorobenzene-d4	11.822

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	91
5			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042122.D
Acq On : 20 Jan 2021 22:21
Operator : SY/MD
Sample : M1180-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 31 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E08

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.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...	7.179	0.6	ug/L	31362	1	6.256	272945	5.0
2-Hexanone, 5-m...	10.243	0.5	ug/L	36142	2	9.427	340045	5.0
1-Hexanol, 2-et...	12.070	3.7	ug/L	249837	3	11.822	341129	5.0
2,4-Octanedione	14.201	0.7	ug/L	47592	3	11.822	341129	5.0
Butylated Hydro...	16.899	2.1	ug/L	141402	3	11.822	341129	5.0