

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
 Data File : VU042116.D
 Acq On : 20 Jan 2021 19:24
 Operator : SY/MD
 Sample : M1180-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F1E03

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: VU042116.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	71	81	89	rVB	57357	69961	13.36%	1.362%
2	1.916	171	179	189	rBV	42970	54105	10.33%	1.054%
3	2.009	201	208	216	rBV	4372	8226	1.57%	0.160%
4	2.568	371	382	395	rBV	83462	132756	25.35%	2.585%
5	3.391	624	638	641	rBV6	3082	7042	1.34%	0.137%
6	4.716	1024	1050	1051	rBV	22271	60880	11.63%	1.186%
7	5.073	1144	1161	1183	rBV2	83982	186045	35.53%	3.623%
8	5.732	1344	1366	1393	rBV2	177222	444519	84.88%	8.657%
9	6.256	1515	1529	1548	rVB	154213	289394	55.26%	5.636%
10	6.700	1654	1667	1683	rBV	103656	202403	38.65%	3.942%
11	7.185	1806	1818	1831	rBV	25011	49999	9.55%	0.974%
12	7.574	1926	1939	1956	rBV	63828	112439	21.47%	2.190%
13	7.906	2030	2042	2057	rVB	210911	362352	69.19%	7.057%
14	8.050	2079	2087	2098	rVB3	4429	8055	1.54%	0.157%
15	8.189	2117	2130	2145	rBV	42219	72940	13.93%	1.420%
16	8.504	2214	2228	2237	rBV4	6784	12973	2.48%	0.253%
17	8.558	2237	2245	2257	rVB8	4606	7302	1.39%	0.142%
18	8.652	2260	2274	2310	rBV	233451	523673	100.00%	10.198%
19	8.799	2310	2320	2332	rVB6	3124	5867	1.12%	0.114%
20	9.426	2502	2515	2543	rBV	211855	363836	69.48%	7.085%
21	9.619	2555	2575	2578	rBV5	4956	10609	2.03%	0.207%
22	9.645	2579	2583	2593	rVB2	6525	9107	1.74%	0.177%
23	9.780	2608	2625	2639	rBV3	7758	17670	3.37%	0.344%
24	9.928	2661	2671	2681	rBV2	11662	18679	3.57%	0.364%
25	10.246	2755	2770	2784	rBV	15201	27531	5.26%	0.536%
26	10.356	2797	2804	2821	rVB4	5516	9960	1.90%	0.194%
27	10.693	2901	2909	2920	rVB	12872	20208	3.86%	0.394%
28	10.767	2920	2932	2947	rBV	82531	134120	25.61%	2.612%
29	10.902	2968	2974	2981	rVB4	3558	5341	1.02%	0.104%
30	10.976	2981	2997	3011	rBV	18263	31698	6.05%	0.617%
31	11.060	3013	3023	3039	rVB5	8021	15366	2.93%	0.299%
32	11.478	3147	3153	3162	rVB4	4968	7393	1.41%	0.144%
33	11.584	3176	3186	3195	rBV3	5319	8907	1.70%	0.173%
34	11.696	3215	3221	3232	rVB5	5063	7814	1.49%	0.152%
35	11.822	3248	3260	3274	rVV	226301	364862	69.67%	7.105%
36	11.899	3276	3284	3296	rVB4	3694	5841	1.12%	0.114%

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37	11.989	3305	3312	3323	rVB3	4456	7053	1.35%	0.137%
38	12.069	3325	3337	3362	rBV	192687	357083	68.19%	6.954%
39	12.201	3367	3378	3397	rVB	209947	347610	66.38%	6.770%
40	12.333	3411	3419	3425	rBV2	10143	14572	2.78%	0.284%
41	12.536	3469	3482	3491	rVB7	4438	9333	1.78%	0.182%
42	12.783	3549	3559	3568	rBV3	8471	13132	2.51%	0.256%
43	12.896	3586	3594	3607	rVB5	6870	9740	1.86%	0.190%
44	12.957	3607	3613	3623	rVB4	4384	5999	1.15%	0.117%
45	13.012	3623	3630	3642	rBV5	4114	6721	1.28%	0.131%
46	13.153	3668	3674	3684	rVB2	4793	7411	1.42%	0.144%
47	13.619	3807	3819	3828	rBV3	8107	12358	2.36%	0.241%
48	14.201	3988	4000	4012	rVB	63514	95505	18.24%	1.860%
49	14.323	4028	4038	4050	rBV4	6663	10632	2.03%	0.207%
50	15.011	4239	4252	4261	rBV6	3635	7597	1.45%	0.148%
51	15.703	4458	4467	4481	rVB5	10109	15757	3.01%	0.307%
52	16.143	4596	4604	4614	rVB3	17175	24095	4.60%	0.469%
53	16.780	4793	4802	4817	rBV2	41266	63852	12.19%	1.243%
54	16.899	4827	4839	4852	rBV2	303812	456619	87.20%	8.892%

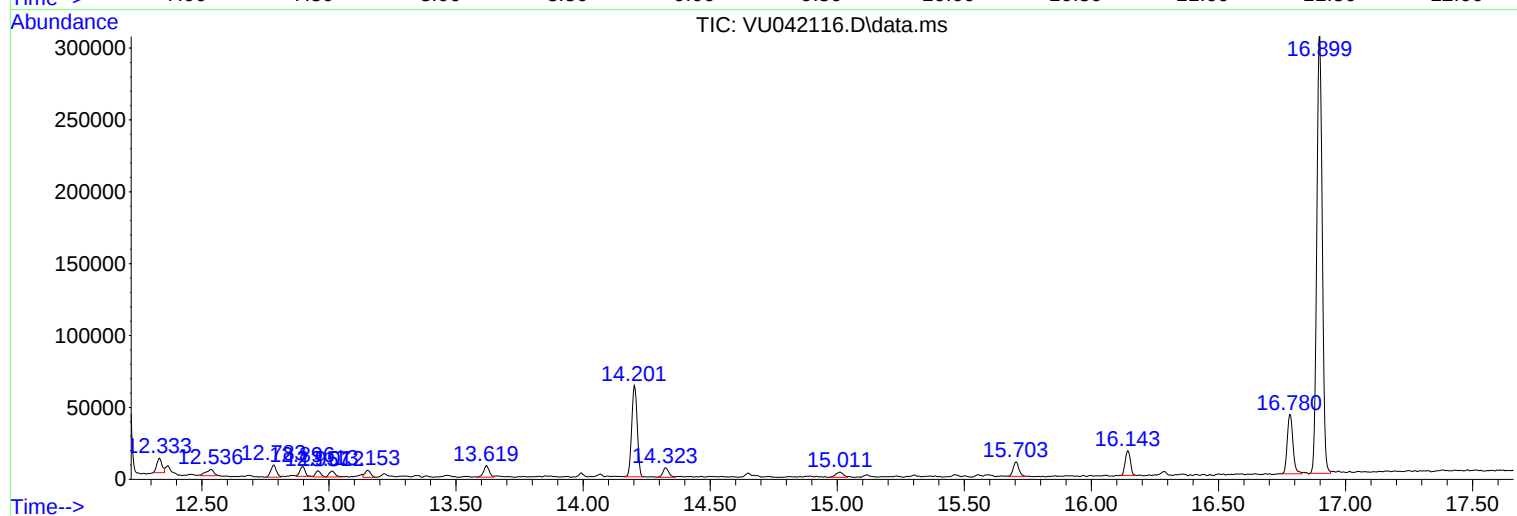
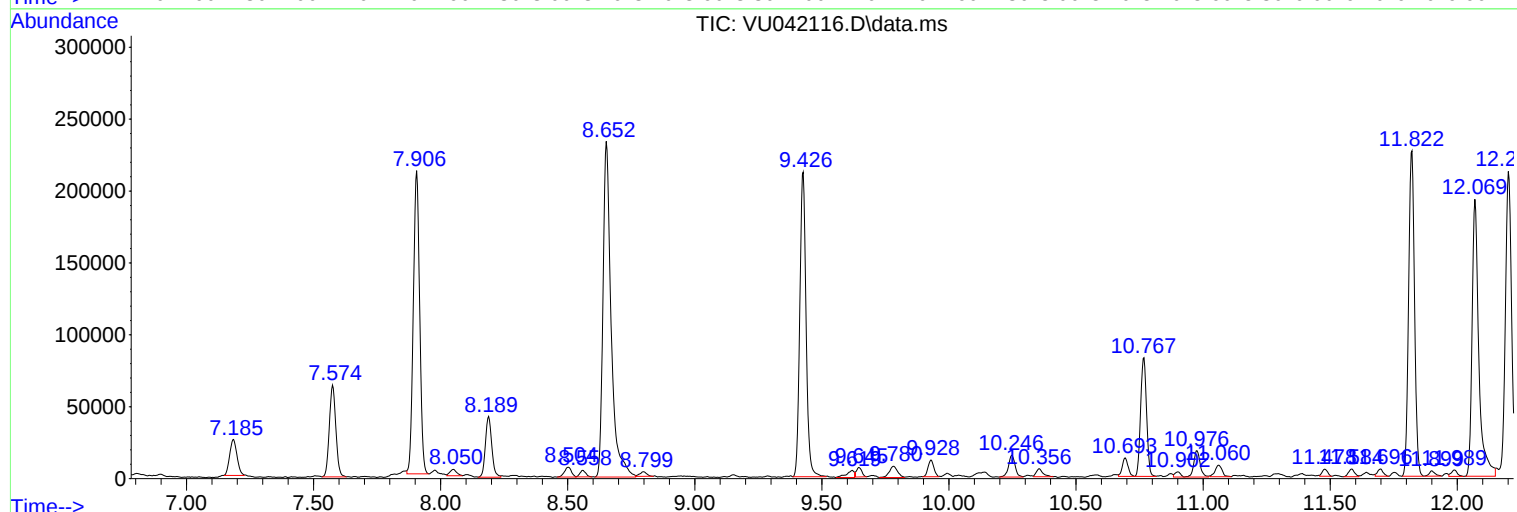
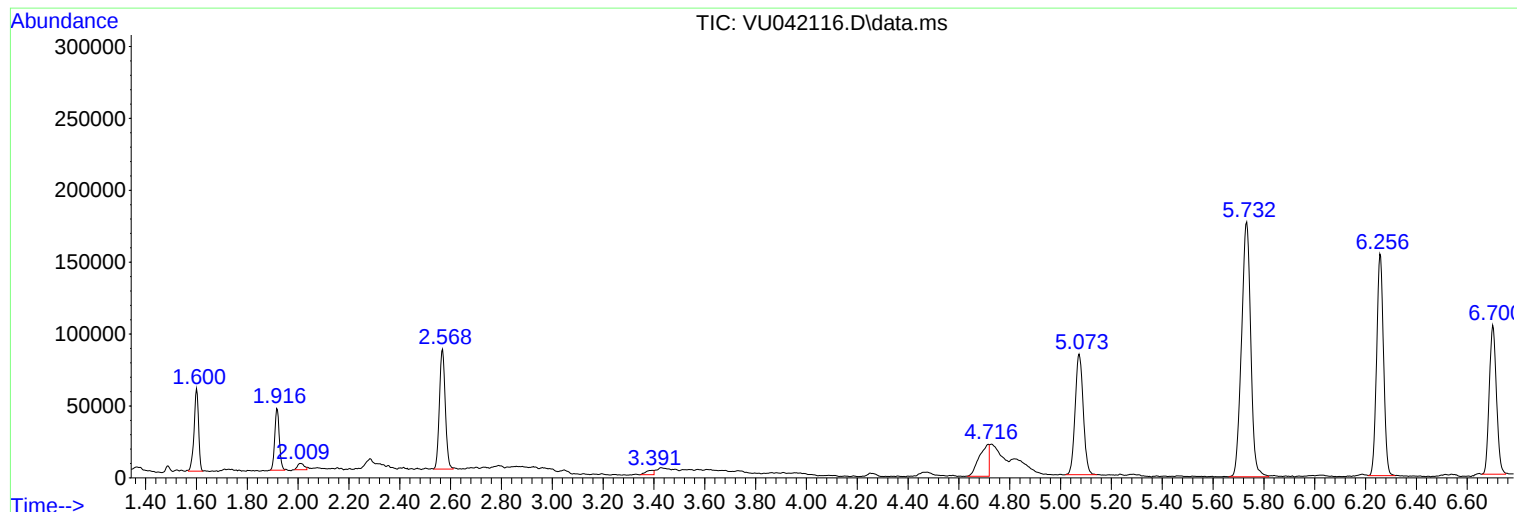
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
MSVOA_U
ClientSampleId :
F1E03

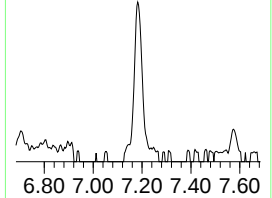
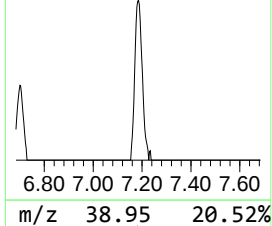
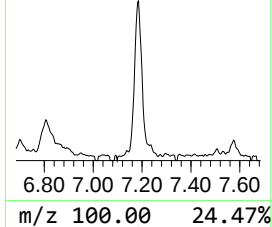
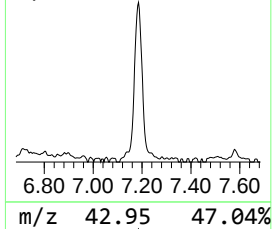
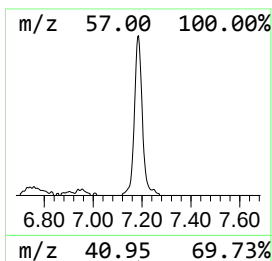
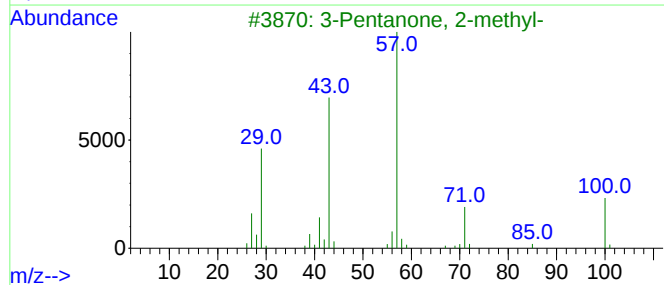
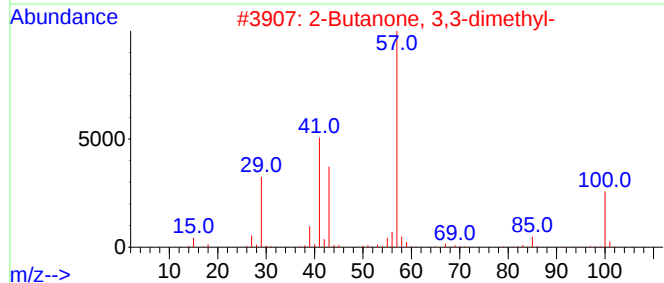
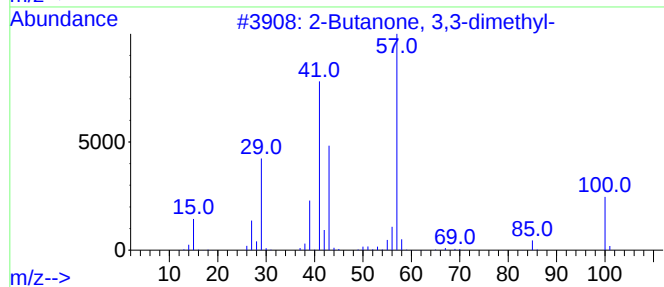
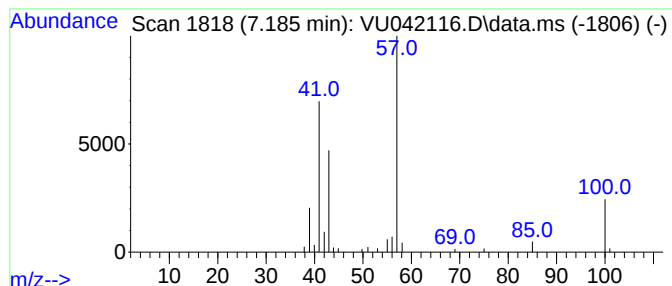
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	0.86 ug/L	49999	1,4-Difluorobenzene	6.259

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	86
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	58
4	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	53
5	3-Hexanone			100	C6H12O	000589-38-8	53



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ALS Vial : 24 Sample Multiplier: 1

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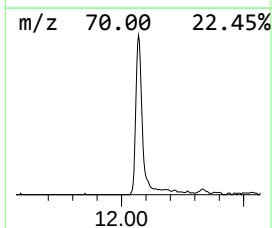
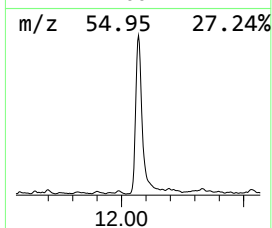
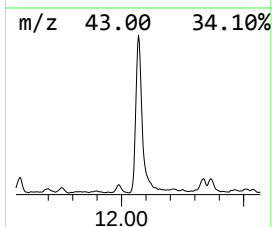
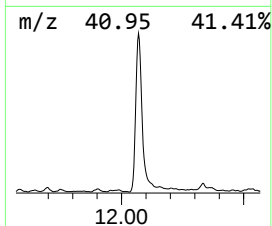
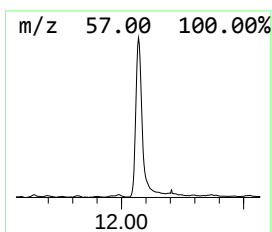
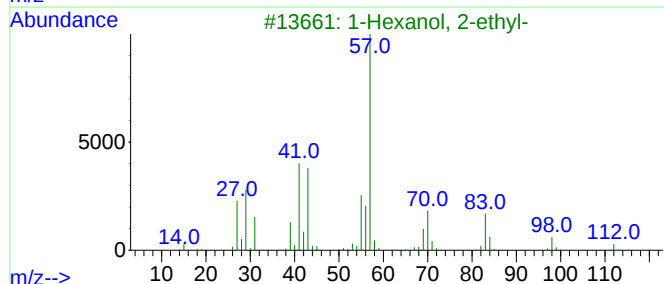
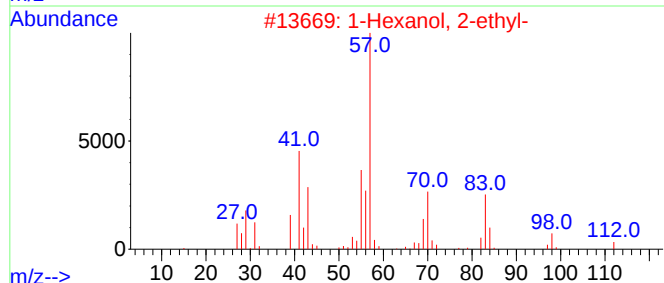
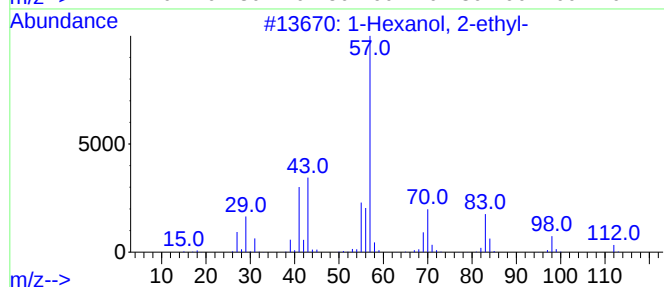
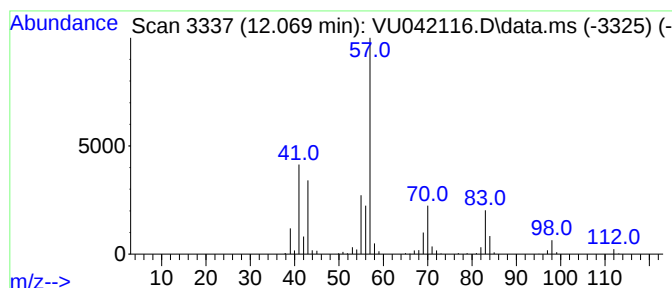
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	4.89 ug/L	357083	1,4-Dichlorobenzene-d4	11.819

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	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	59



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

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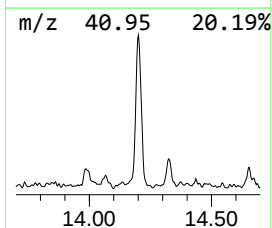
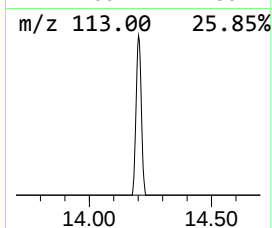
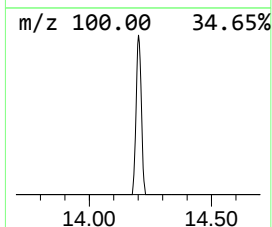
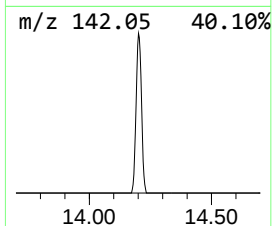
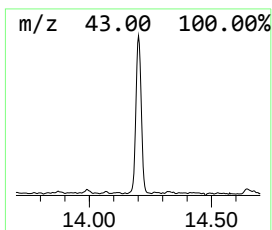
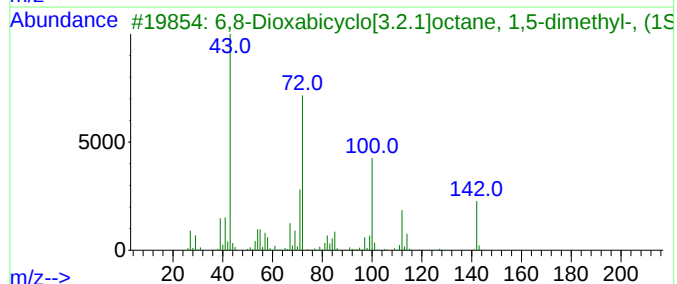
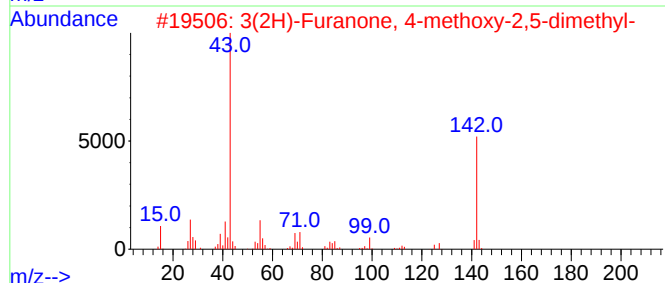
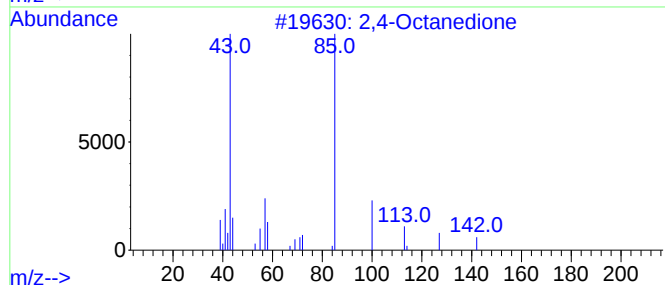
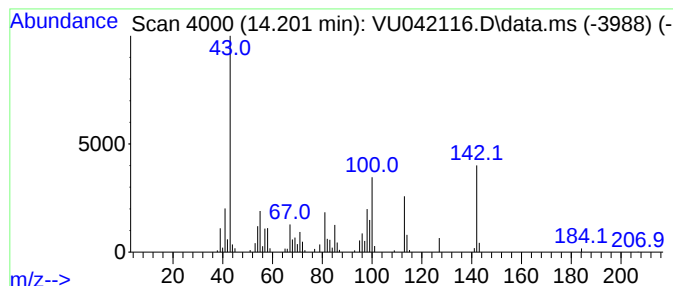
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	1.31 ug/L	95505	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Octanedione		142	C8H14O2	014090-87-0	47	
2	3(2H)-Furanone, 4-methoxy-2,5-di...		142	C7H10O3	004077-47-8	38	
3	6,8-Dioxabicyclo[3.2.1]octane, 1...		142	C8H14O2	028401-39-0	35	
4	4-(7-Methoxy-3,3,7-trimethyl-oxe...		240	C14H24O3	107675-07-0	17	
5	6-Dodecanone		184	C12H24O	006064-27-3	12	



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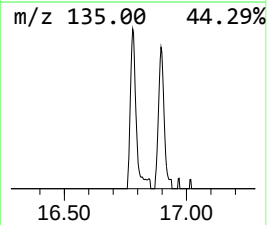
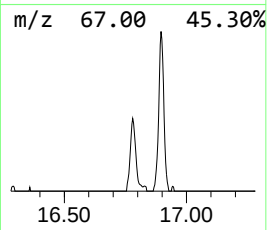
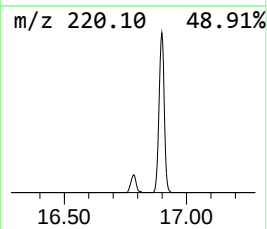
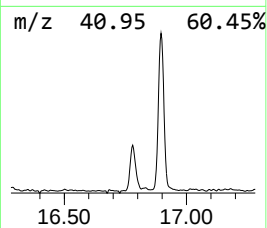
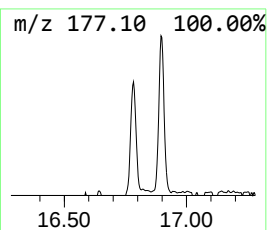
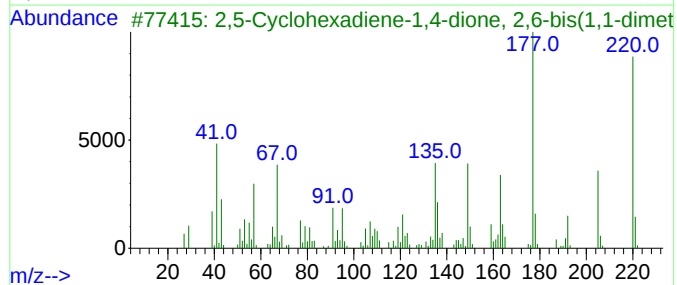
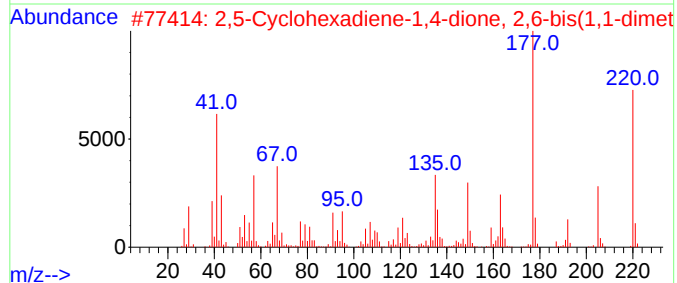
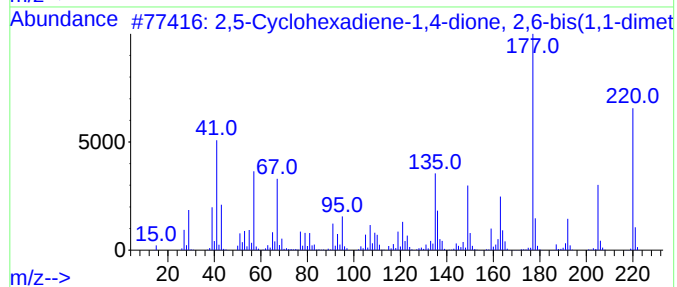
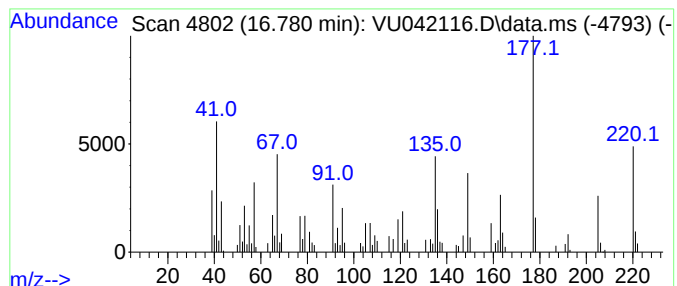
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.780	0.88 ug/L	63852	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	64
4			Thiocoumarin, 4,4,6,8-tetramethyl-	220	C13H16OS	1000128-90-3	43
5			trans-.beta.-Ionone	192	C13H20O	000079-77-6	38



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F1E03

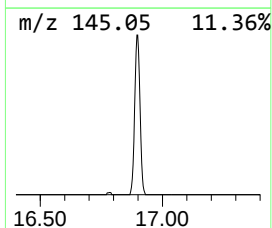
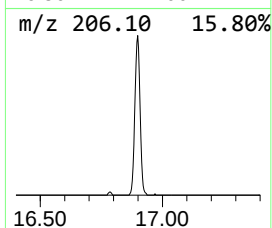
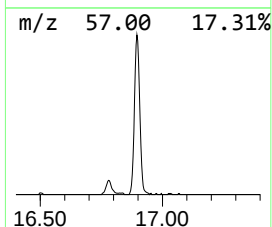
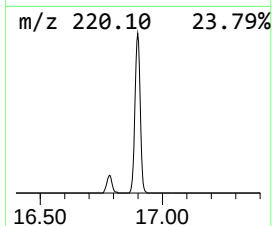
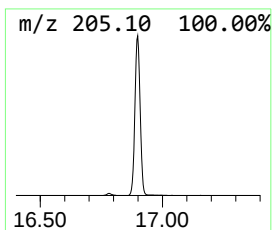
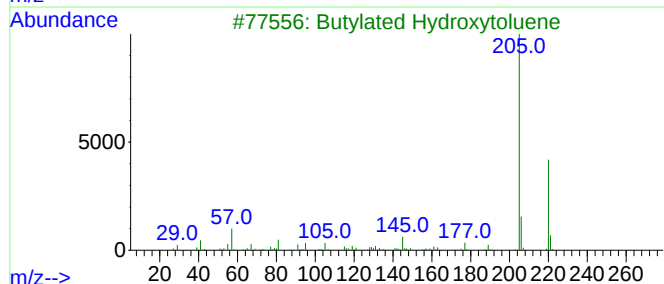
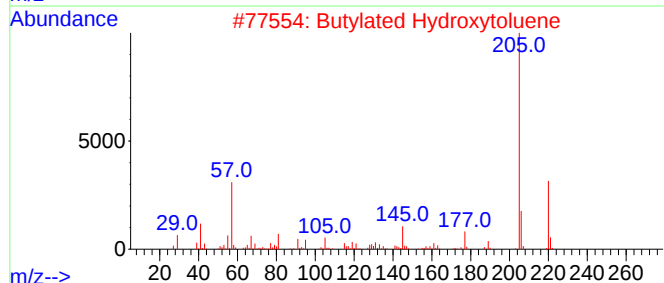
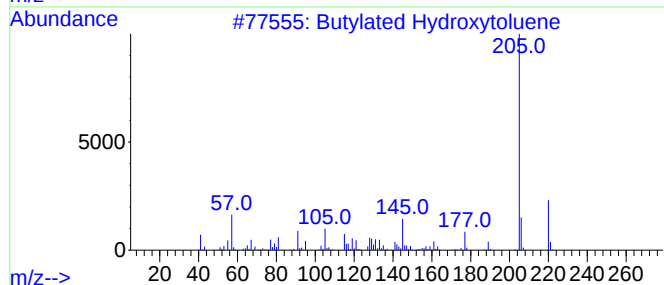
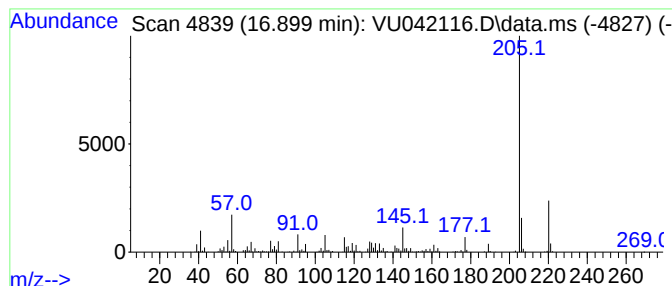
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Quant Title : TRACE VOA SOM01.0

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.
16.899	6.26 ug/L	456619	1,4-Dichlorobenzene-d4	11.819

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	93
5			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042116.D
Acq On : 20 Jan 2021 19:24
Operator : SY/MD
Sample : M1180-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E03

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...	7.185	0.9	ug/L	49999	1	6.259	289394	5.0
1-Hexanol, 2-et...	12.069	4.9	ug/L	357083	3	11.819	364862	5.0
unknown-01	14.201	1.3	ug/L	95505	3	11.819	364862	5.0
2,5-Cyclohexadi...	16.780	0.9	ug/L	63852	3	11.819	364862	5.0
Butylated Hydro...	16.899	6.3	ug/L	456619	3	11.819	364862	5.0