

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042173.D
 Acq On : 22 Jan 2021 16:34
 Operator : SY/MD
 Sample : M1222-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :

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: VU042173.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	93	rVB	43381	52669	10.61%	1.242%
2	1.919	171	180	189	rBV	33787	42441	8.55%	1.000%
3	2.372	315	321	329	rBV	5143	5896	1.19%	0.139%
4	2.568	372	382	397	rVB	76206	121707	24.51%	2.869%
5	3.285	589	605	608	rBV3	4375	8724	1.76%	0.206%
6	4.459	957	970	986	rBV5	2418	5754	1.16%	0.136%
7	4.665	1016	1034	1054	rBV2	52801	168461	33.93%	3.971%
8	5.073	1143	1161	1179	rBV2	70314	155130	31.24%	3.657%
9	5.732	1346	1366	1399	rBV2	138059	359429	72.39%	8.473%
10	6.256	1515	1529	1555	rVB	133004	245879	49.52%	5.796%
11	6.700	1654	1667	1689	rVB	89709	174546	35.15%	4.115%
12	7.176	1802	1815	1835	rVB	19179	40909	8.24%	0.964%
13	7.574	1927	1939	1959	rVB	51583	90797	18.29%	2.140%
14	7.835	2002	2020	2030	rBV8	4609	13034	2.63%	0.307%
15	7.906	2030	2042	2058	rVB	168036	290729	58.55%	6.854%
16	8.044	2076	2085	2095	rVB3	3470	6674	1.34%	0.157%
17	8.189	2119	2130	2143	rBV	33198	56035	11.29%	1.321%
18	8.500	2214	2227	2239	rBV4	2923	6012	1.21%	0.142%
19	8.645	2259	2272	2312	rBV	245871	496530	100.00%	11.705%
20	9.423	2502	2514	2531	rBV	183649	308349	62.10%	7.269%
21	9.648	2576	2584	2594	rVB2	11909	17565	3.54%	0.414%
22	9.774	2607	2623	2633	rBV4	3304	7456	1.50%	0.176%
23	10.243	2759	2769	2779	rBV3	3050	5088	1.02%	0.120%
24	10.349	2794	2802	2811	rBV2	4466	7208	1.45%	0.170%
25	10.764	2920	2931	2943	rBV	71213	115781	23.32%	2.729%
26	10.976	2989	2997	3009	rVB	3974	6833	1.38%	0.161%
27	11.693	3210	3220	3230	rBV2	13043	19577	3.94%	0.461%
28	11.819	3247	3259	3274	rVV	211890	328381	66.14%	7.741%
29	12.073	3327	3338	3362	rBV	16332	35332	7.12%	0.833%
30	12.201	3362	3378	3394	rVB	181677	294341	59.28%	6.939%
31	12.330	3409	3418	3427	rBV2	8823	12701	2.56%	0.299%
32	12.896	3583	3594	3607	rBV3	49489	74725	15.05%	1.762%
33	14.201	3985	4000	4010	rBV2	25297	37521	7.56%	0.885%
34	14.327	4029	4039	4048	rBV5	4030	6884	1.39%	0.162%
35	15.703	4456	4467	4479	rBV3	15898	26031	5.24%	0.614%
36	16.143	4593	4604	4613	rBV2	10159	14253	2.87%	0.336%

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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	16.786	4793	4804	4824	rBV2	66822	122513	24.67%	2.888%
38	16.899	4828	4839	4857	rVB	306552	460143	92.67%	10.847%

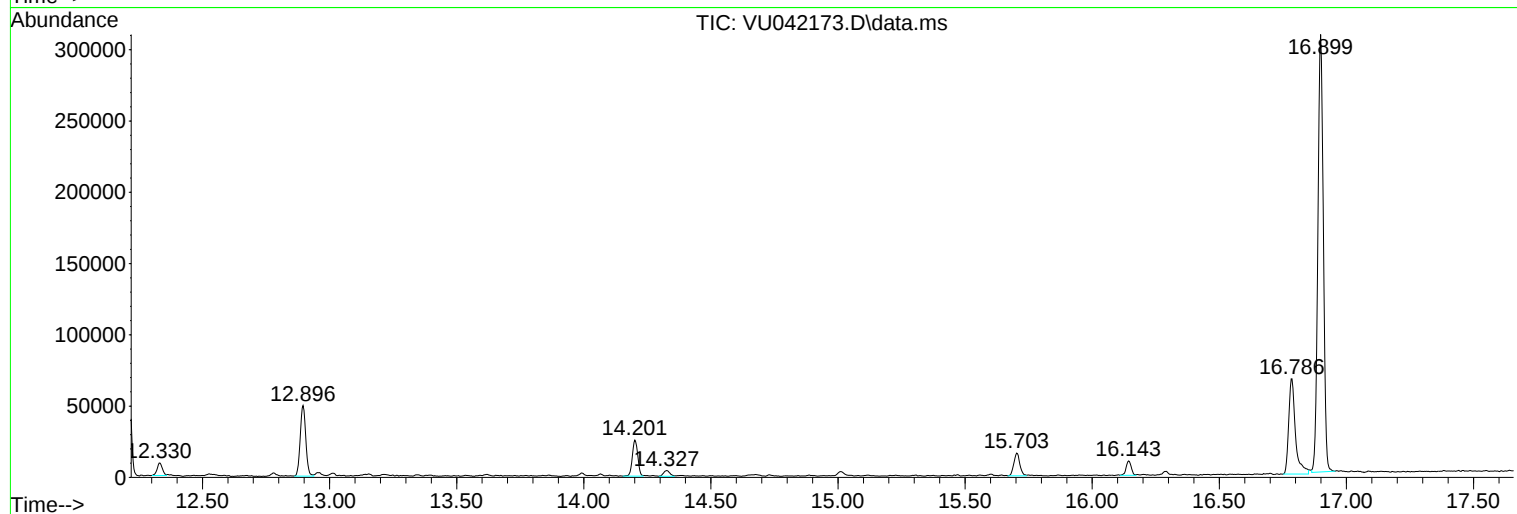
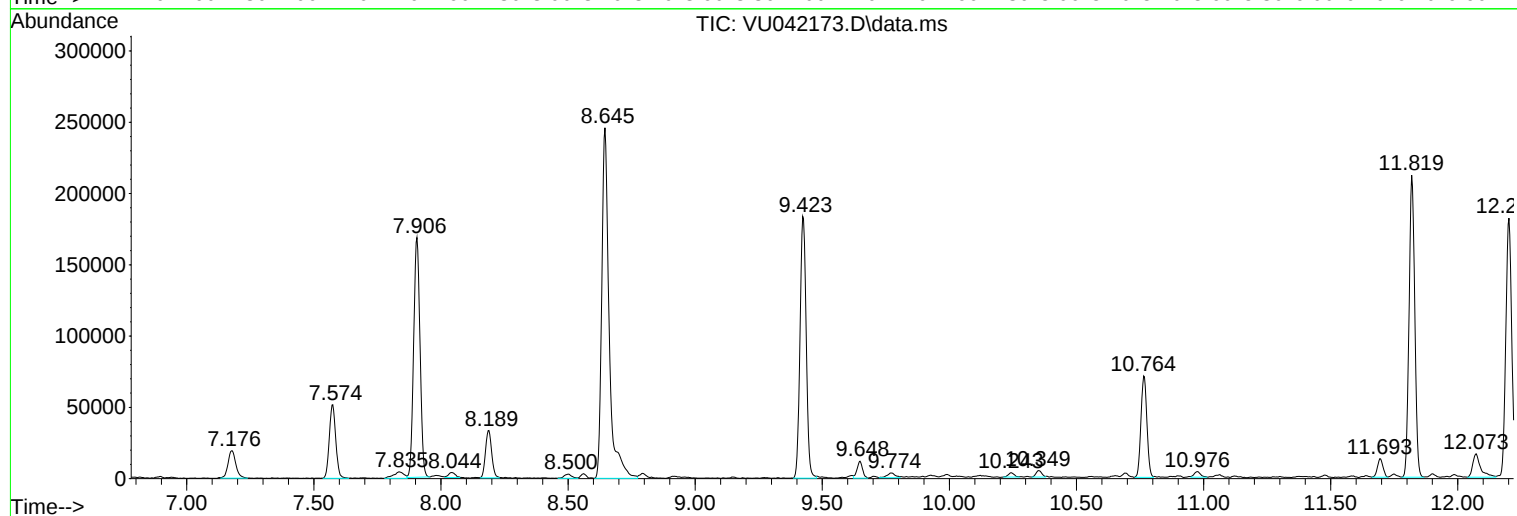
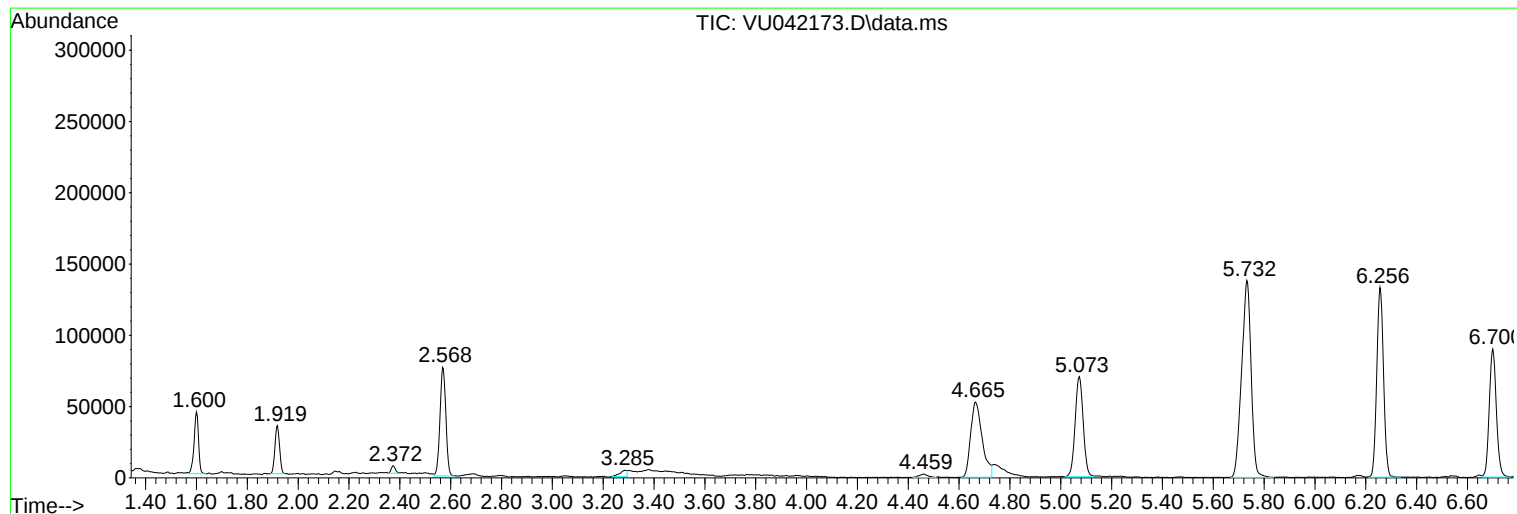
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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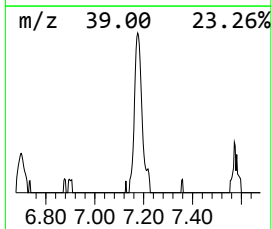
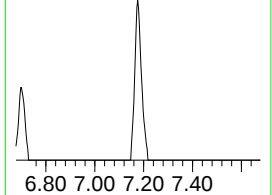
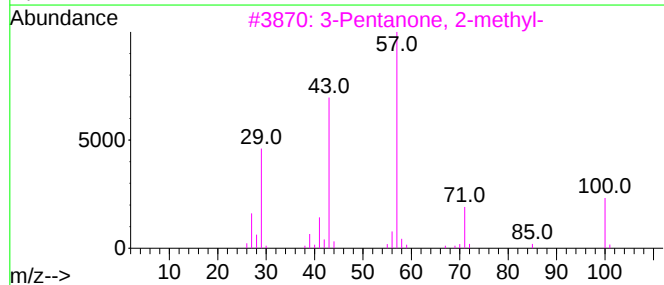
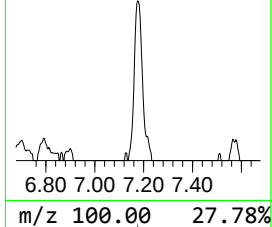
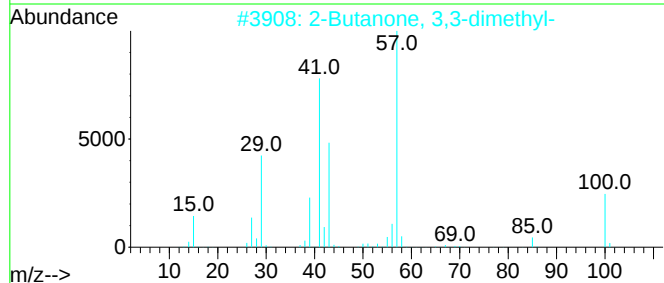
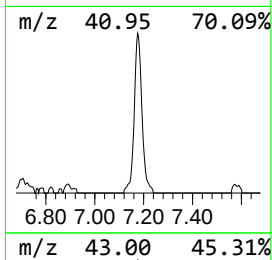
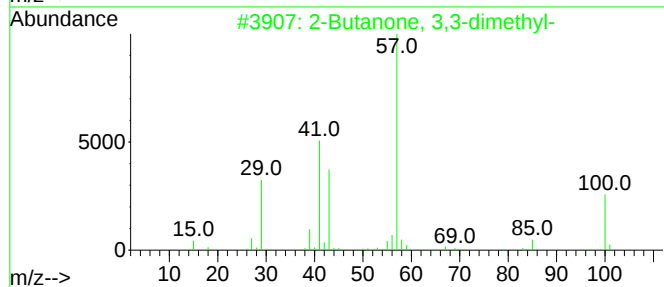
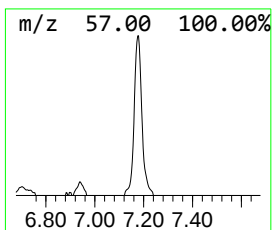
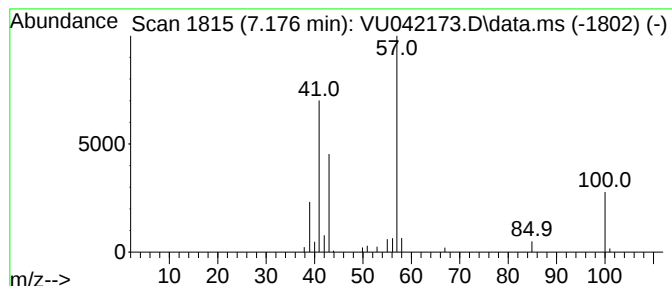
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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.
7.176	0.83 ug/L	40909	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	80
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	64
4	Diazene, bis(1,1-dimethylethyl)-			142	C8H18N2	000927-83-3	47
5	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	40



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ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :

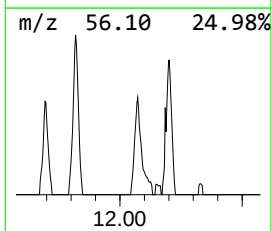
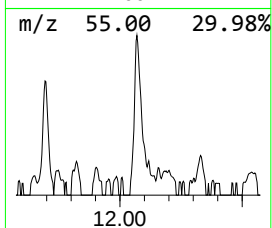
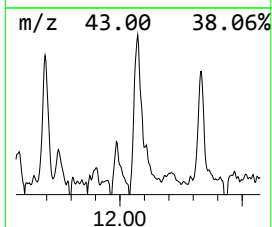
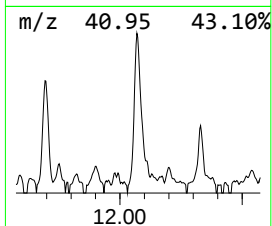
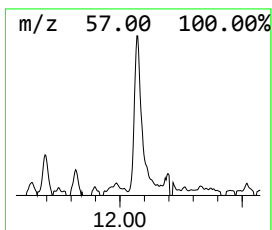
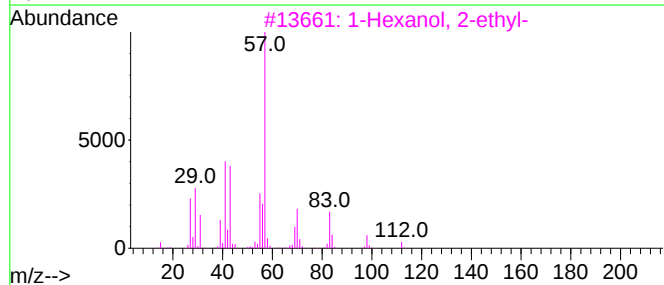
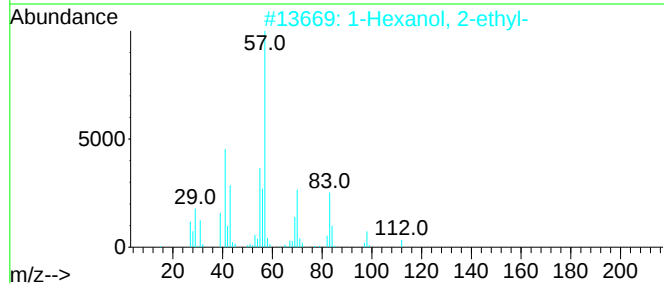
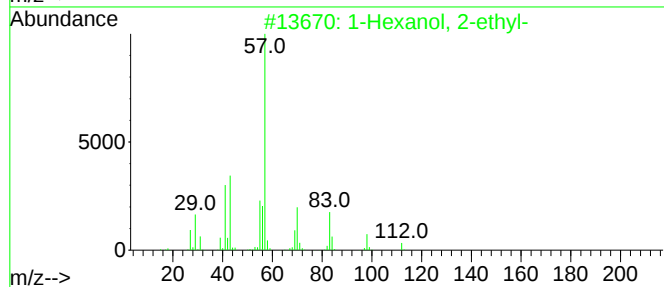
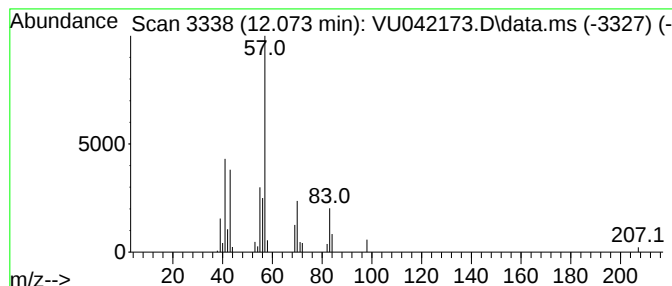
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.073	0.54 ug/L	35332	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	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59



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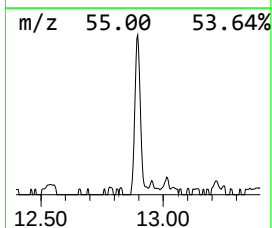
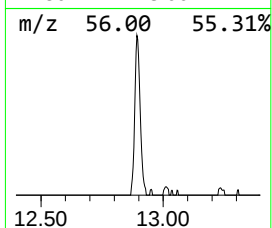
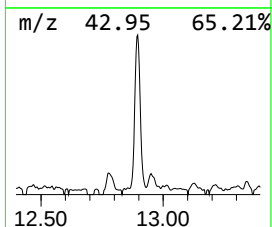
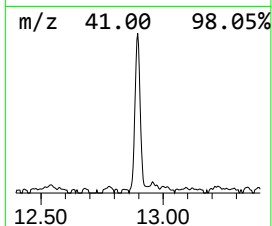
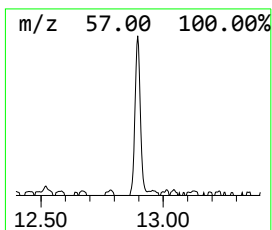
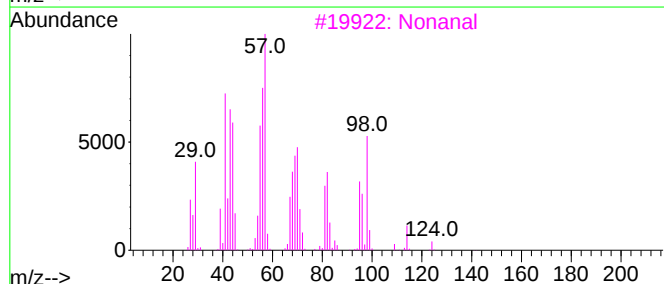
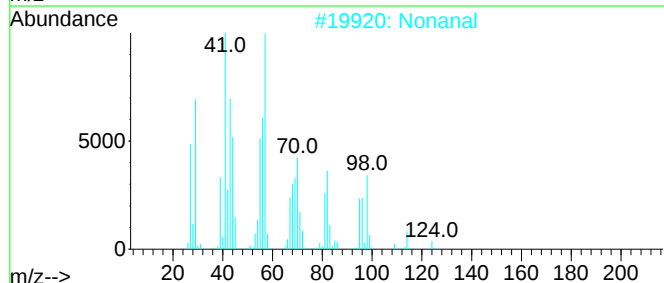
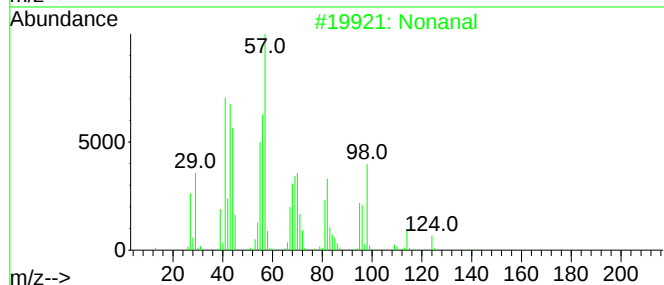
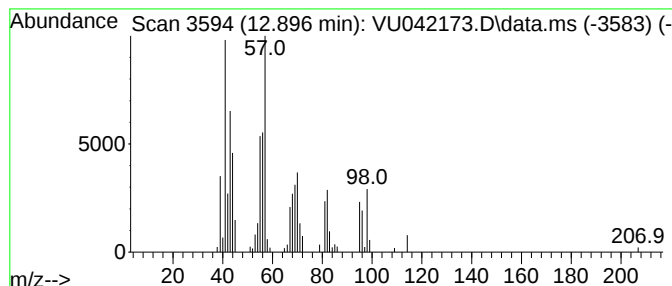
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.896	1.14 ug/L	74725	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal			142	C9H18O	000124-19-6	91
2	Nonanal			142	C9H18O	000124-19-6	91
3	Nonanal			142	C9H18O	000124-19-6	90
4	Nonanal			142	C9H18O	000124-19-6	80
5	2-Nonen-1-ol, (E)-			142	C9H18O	031502-14-4	38



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Instrument :
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ClientSampleId :

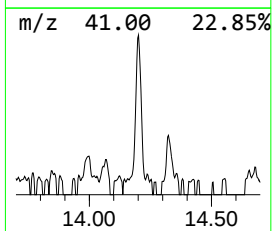
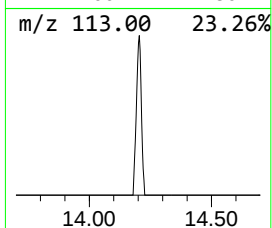
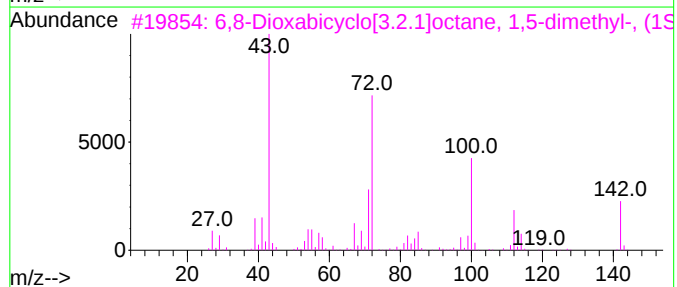
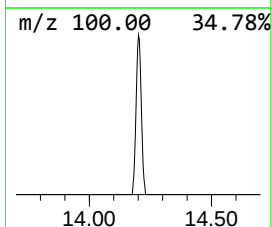
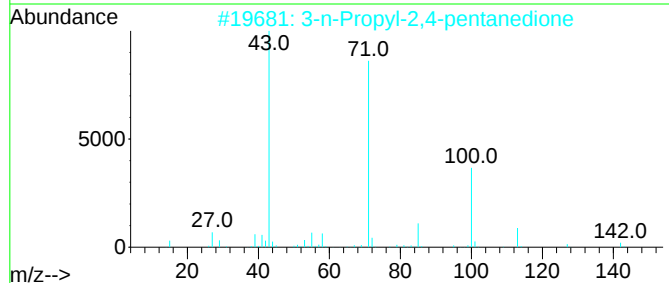
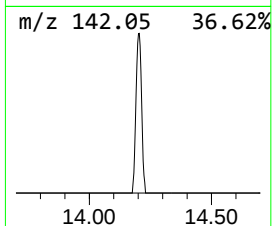
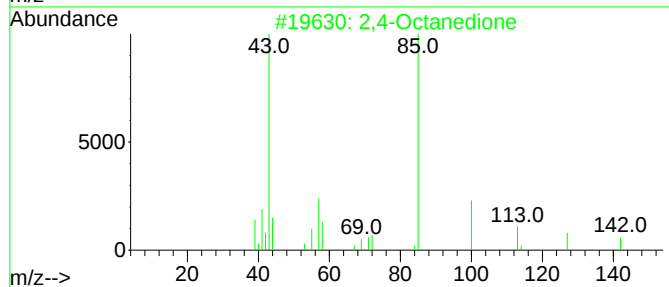
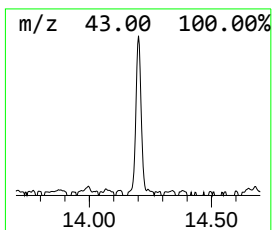
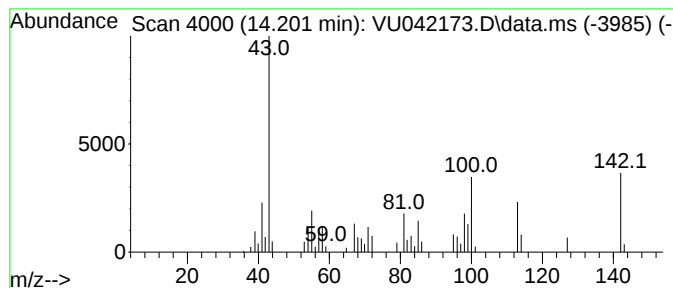
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	0.57 ug/L	37521	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	38
2			3-n-Propyl-2,4-pentanedione	142	C8H14O2	001540-35-8	37
3			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	35
4			5-Undecanone, 2-methyl-	184	C12H24O	050639-02-6	25
5			6-Dodecanone	184	C12H24O	006064-27-3	25



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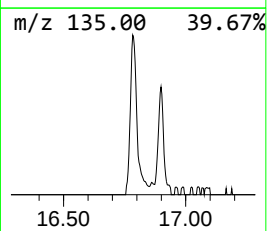
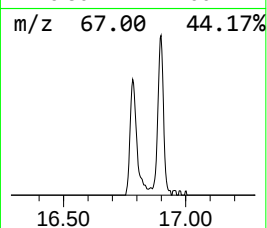
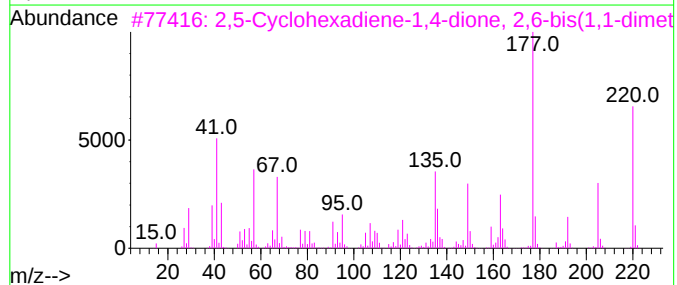
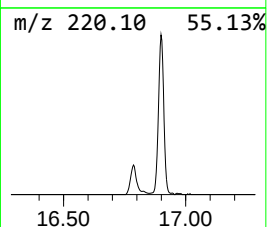
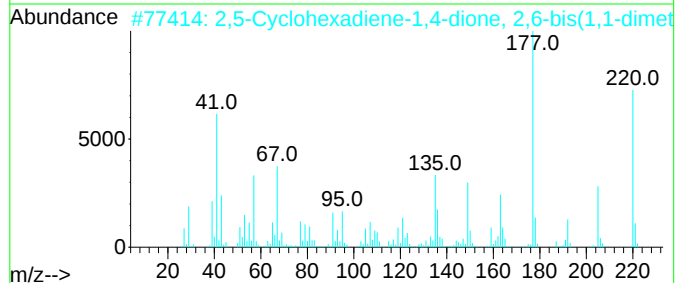
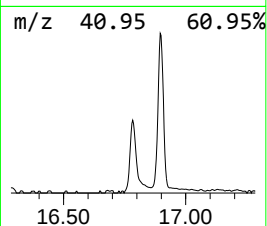
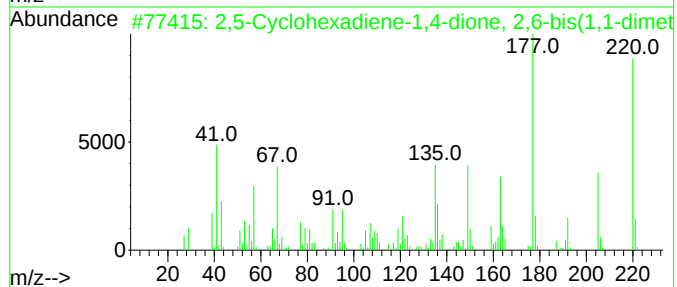
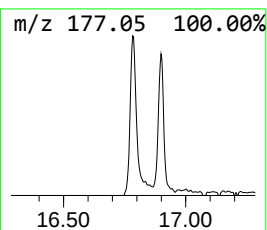
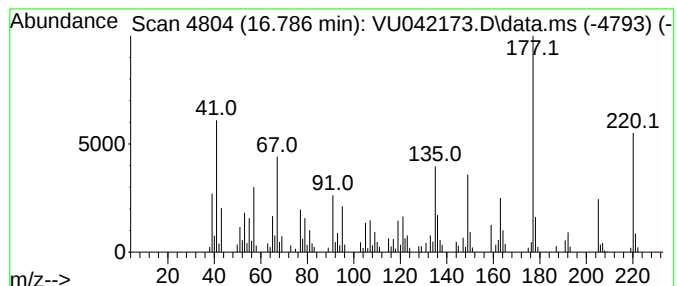
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.786	1.87 ug/L	122513	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	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	90
4			N-[4-(Ethyl-methyl-amino)-phenyl]...	192	C11H16N2O	099981-45-0	43
5			trans-.beta.-Ionone	192	C13H20O	000079-77-6	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042173.D
Acq On : 22 Jan 2021 16:34
Operator : SY/MD
Sample : M1222-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :

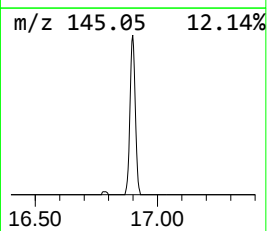
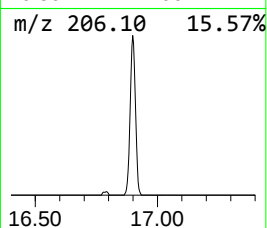
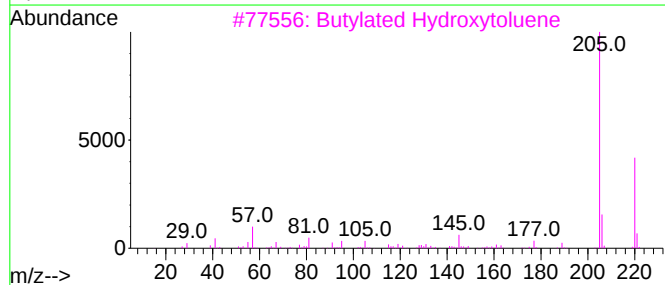
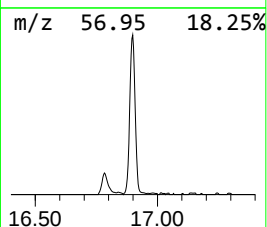
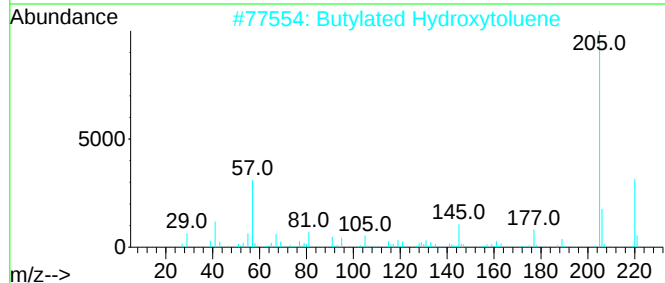
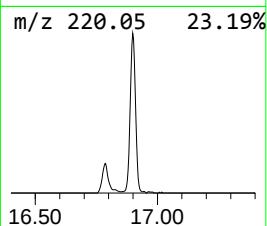
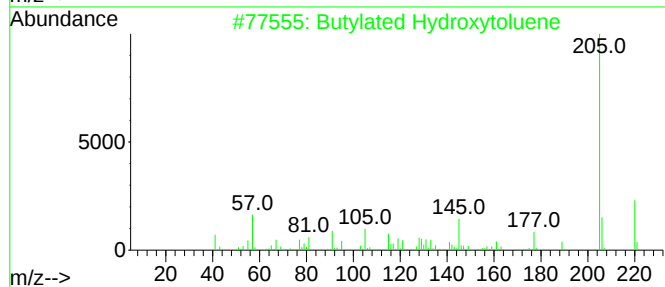
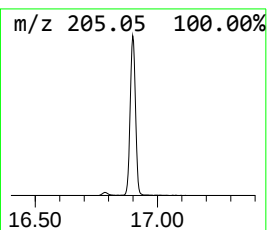
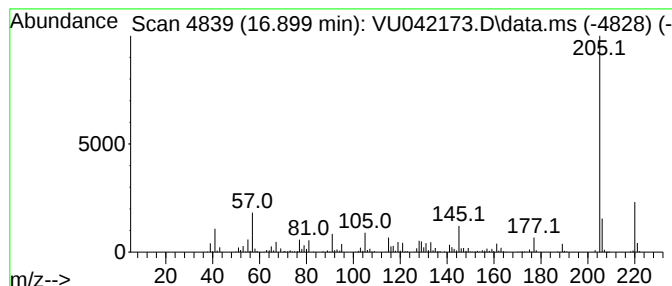
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	7.01 ug/L	460143	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	96
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
5			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042173.D
Acq On : 22 Jan 2021 16:34
Operator : SY/MD
Sample : M1222-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :

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...	7.176	0.8	ug/L	40909	1	6.256	245879	5.0
1-Hexanol, 2-et...	12.073	0.5	ug/L	35332	3	11.819	328381	5.0
Nonanal	12.896	1.1	ug/L	74725	3	11.819	328381	5.0
unknown-01	14.201	0.6	ug/L	37521	3	11.819	328381	5.0
2,5-Cyclohexadi...	16.786	1.9	ug/L	122513	3	11.819	328381	5.0
Butylated Hydro...	16.899	7.0	ug/L	460143	3	11.819	328381	5.0