

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042177.D
 Acq On : 22 Jan 2021 18:10
 Operator : SY/MD
 Sample : M1222-12
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 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: VU042177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	17	rVB2	9117	9089	1.31%	0.199%
2	1.459	23	37	42	rBV	5663	13446	1.93%	0.294%
3	1.591	68	78	89	rVB2	43605	59040	8.49%	1.293%
4	1.909	169	177	188	rVB	33650	41998	6.04%	0.920%
5	2.562	370	380	392	rBV	65678	104229	14.99%	2.282%
6	4.706	1024	1047	1094	rBV2	41558	205064	29.50%	4.490%
7	5.070	1145	1160	1178	rBV	70178	151523	21.80%	3.318%
8	5.729	1346	1365	1382	rBV2	147051	354418	50.98%	7.760%
9	6.256	1516	1529	1545	rVB	131249	245604	35.33%	5.378%
10	6.700	1654	1667	1692	rBV	87752	173460	24.95%	3.798%
11	7.185	1805	1818	1834	rVB	38056	74974	10.78%	1.642%
12	7.571	1925	1938	1950	rBV	51014	88790	12.77%	1.944%
13	7.809	2003	2012	2017	rBV2	5687	9272	1.33%	0.203%
14	7.851	2018	2025	2031	rVV2	12256	23394	3.37%	0.512%
15	7.902	2031	2041	2055	rVB	170838	294096	42.30%	6.439%
16	8.047	2078	2086	2099	rVB3	6032	10764	1.55%	0.236%
17	8.189	2119	2130	2142	rBV	33394	55703	8.01%	1.220%
18	8.504	2216	2228	2236	rBV2	6063	10714	1.54%	0.235%
19	8.558	2236	2245	2255	rVB4	12542	20108	2.89%	0.440%
20	8.648	2260	2273	2308	rBV	247107	479676	69.00%	10.503%
21	9.423	2501	2514	2534	rBV	189056	309731	44.55%	6.782%
22	9.648	2564	2584	2595	rVB3	17893	31342	4.51%	0.686%
23	9.774	2611	2623	2638	rVB4	6047	12539	1.80%	0.275%
24	9.928	2661	2671	2681	rVB2	7787	12517	1.80%	0.274%
25	10.690	2903	2908	2920	rVB2	7441	10988	1.58%	0.241%
26	10.764	2920	2931	2945	rBV	70960	111830	16.09%	2.449%
27	10.973	2987	2996	3012	rVB2	7904	13666	1.97%	0.299%
28	11.475	3141	3152	3163	rVB6	5265	10233	1.47%	0.224%
29	11.819	3246	3259	3275	rVB	209480	324546	46.68%	7.106%
30	12.070	3324	3337	3364	rBV	36723	82803	11.91%	1.813%
31	12.201	3366	3378	3392	rVB	177328	284292	40.89%	6.225%
32	12.330	3410	3418	3428	rBV2	7872	12286	1.77%	0.269%
33	14.201	3986	4000	4011	rBV	59277	87805	12.63%	1.923%
34	15.703	4458	4467	4479	rVB5	18812	29226	4.20%	0.640%
35	16.143	4595	4604	4615	rVB2	23866	34579	4.97%	0.757%
36	16.783	4792	4803	4821	rBV3	47202	78264	11.26%	1.714%

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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	16.899	4825	4839	4859	rBV	458271	695208	100.00%	15.222%
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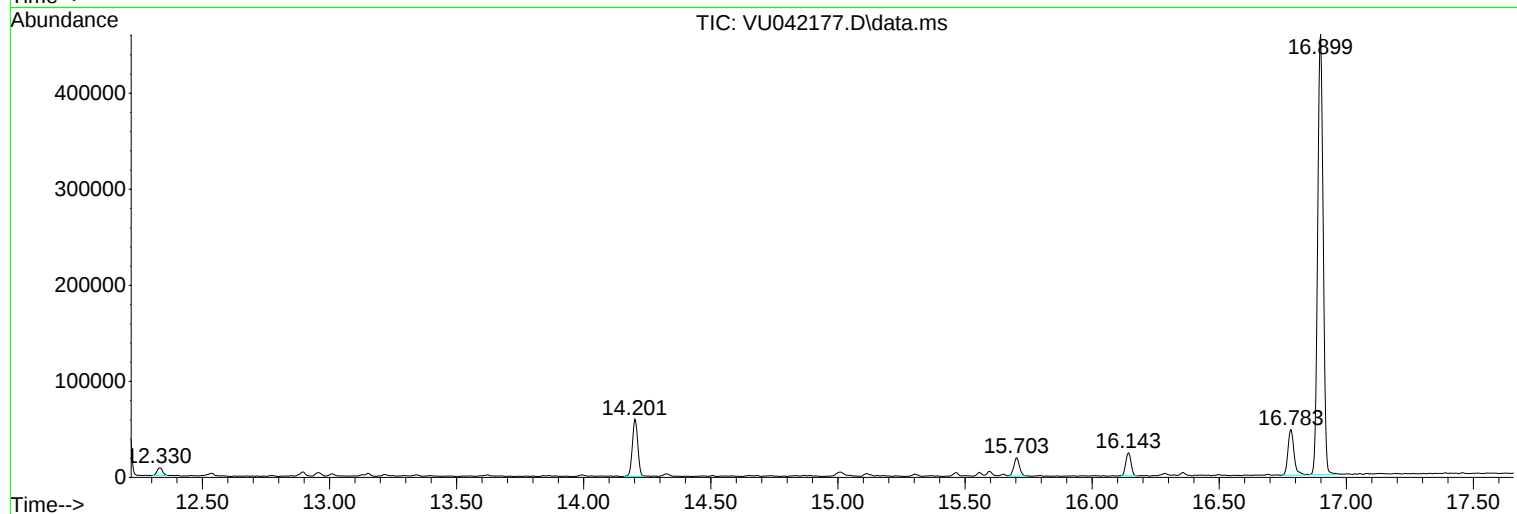
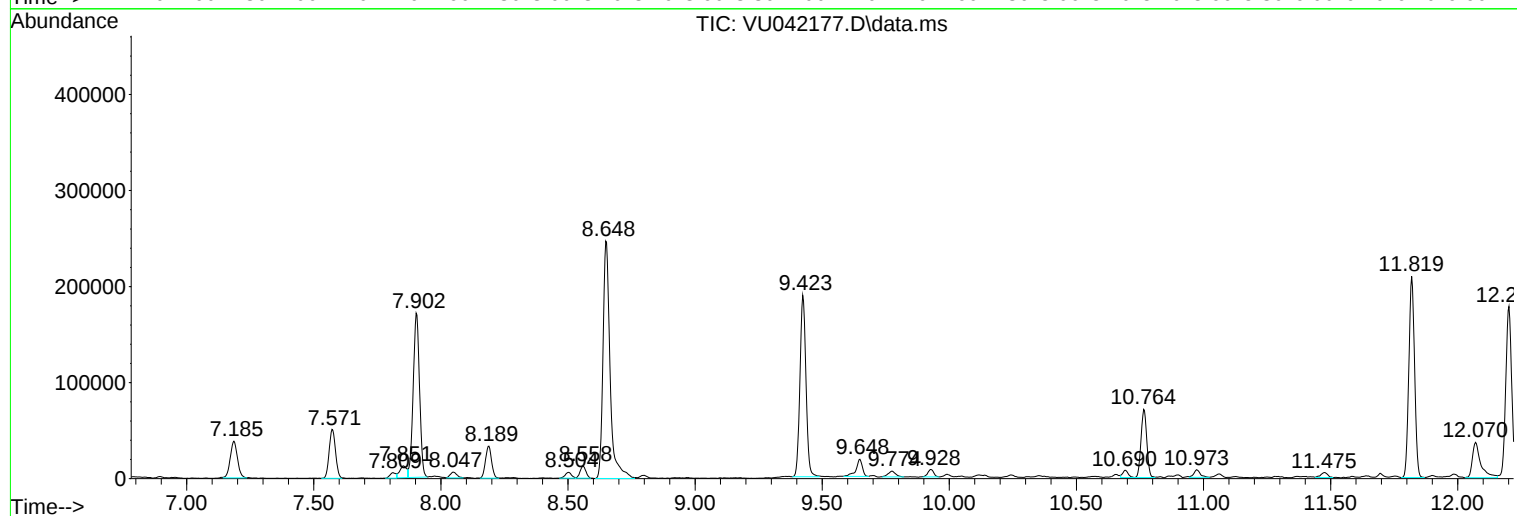
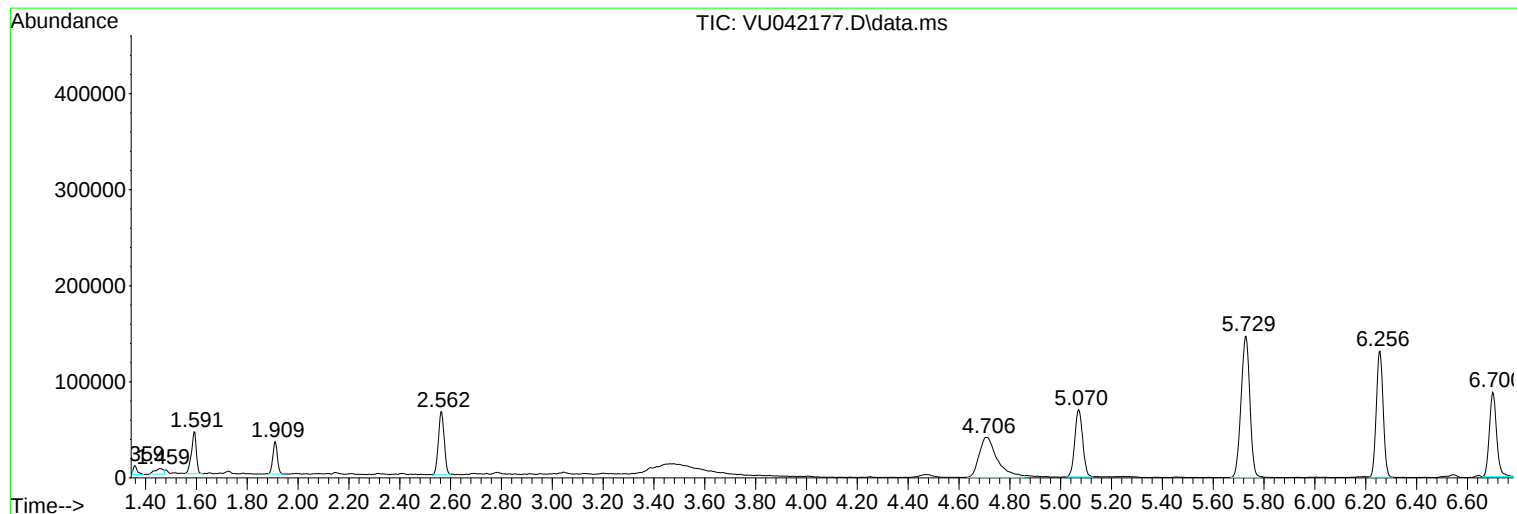
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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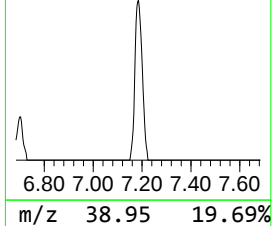
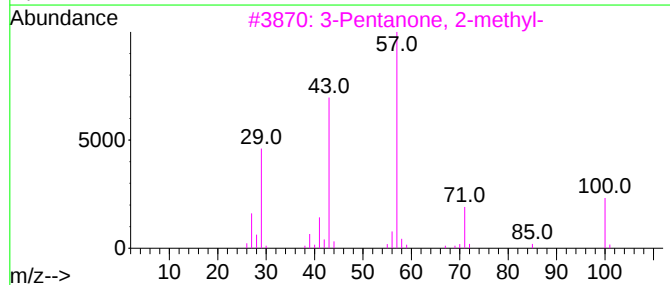
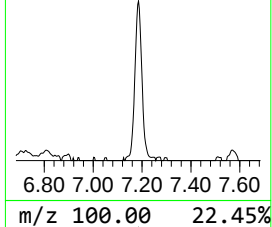
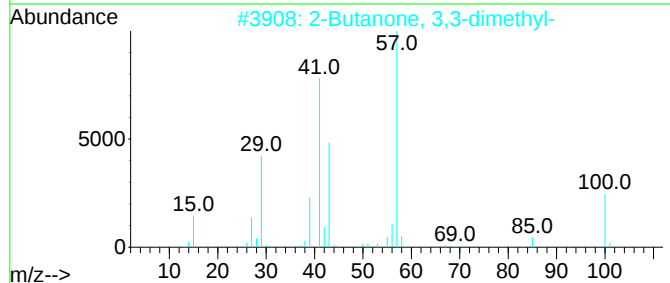
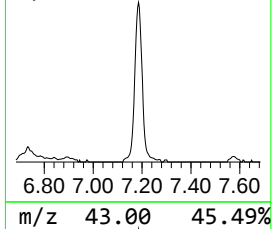
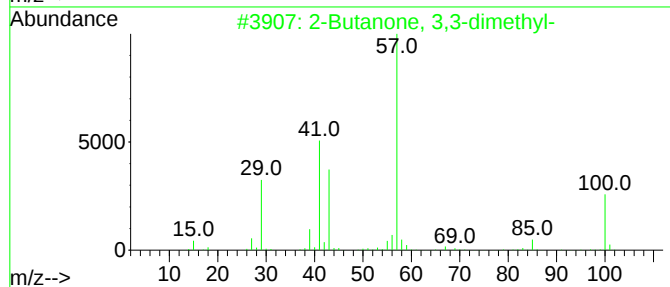
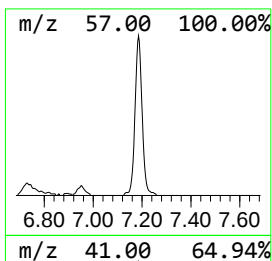
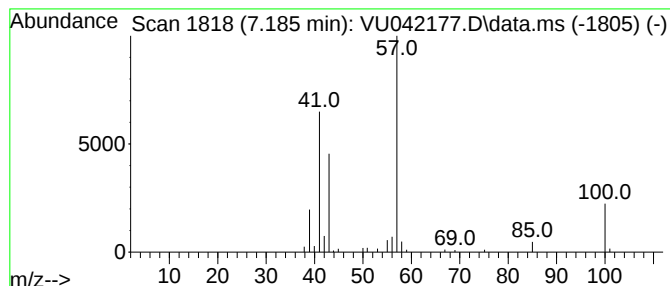
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.185	1.53 ug/L	74974	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	86
2	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	83
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	80
4	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	72
5	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	59



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Instrument :
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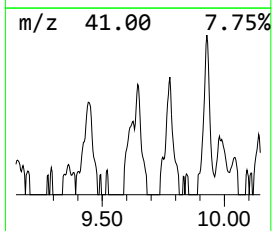
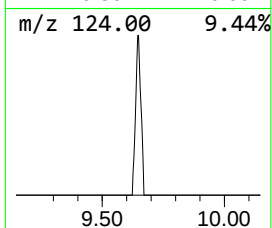
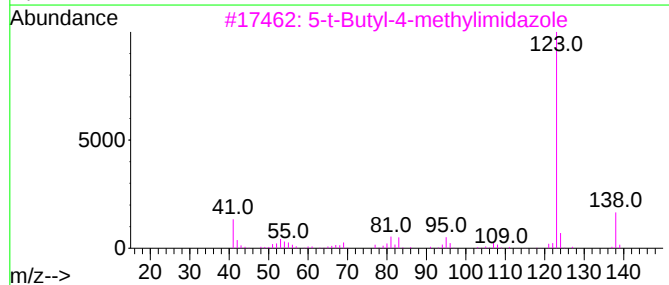
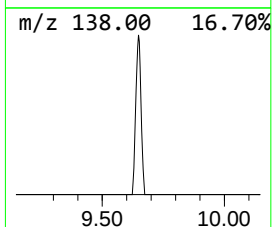
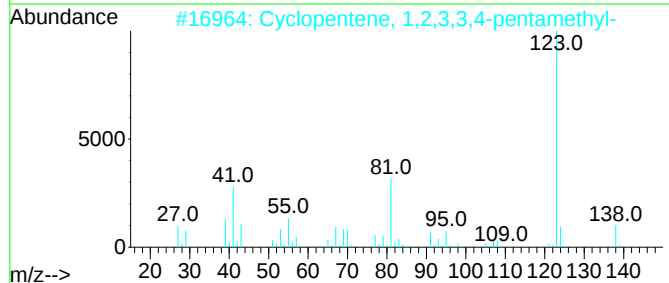
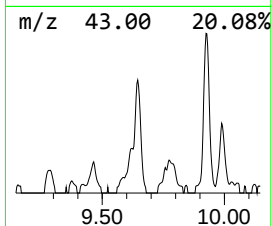
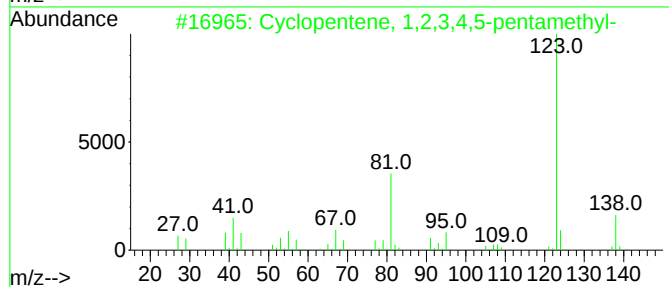
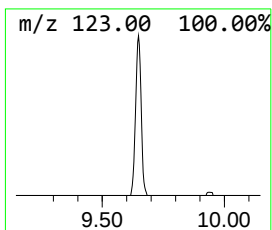
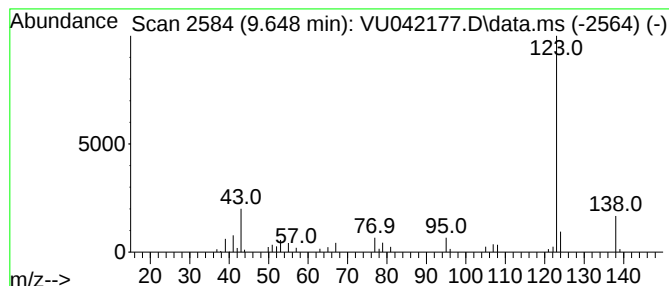
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Cyclopentene, 1,2,3,4,5-pen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.648	0.51 ug/L	31342	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,2,3,4,5-pentamet...	138	C10H18	1000154-28-6	91
2			Cyclopentene, 1,2,3,3,4-pentamet...	138	C10H18	197390-29-7	90
3			5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	78
4			Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	78
5			1-(1-Ethyl-2,3-dimethyl-cyclopen...	166	C11H18O	1000185-18-6	72



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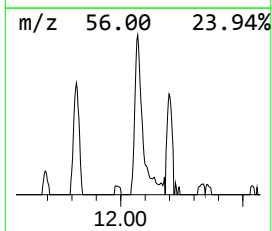
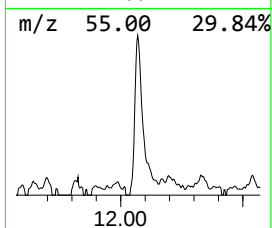
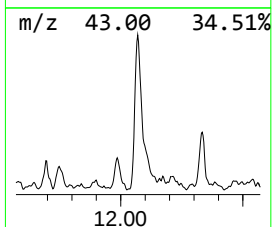
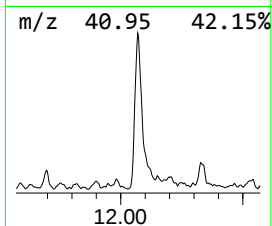
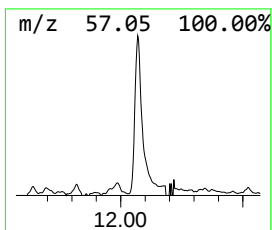
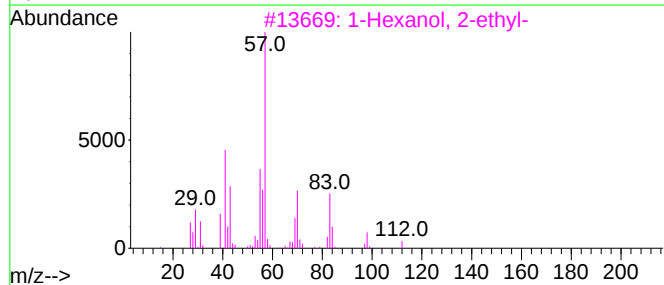
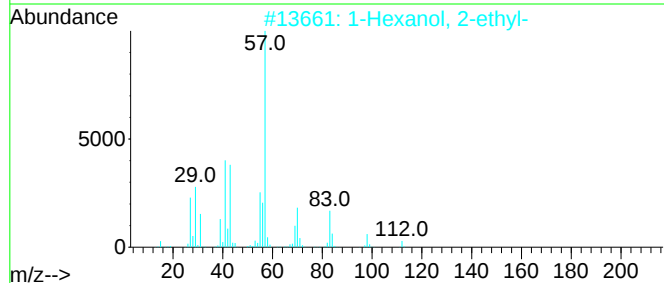
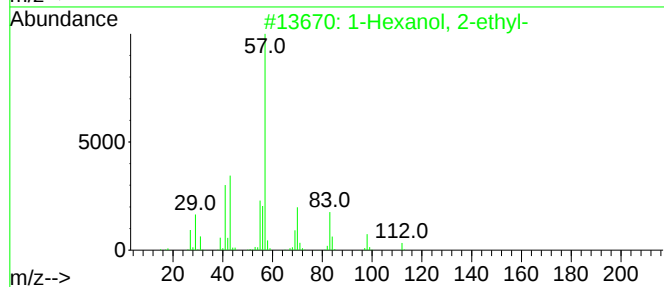
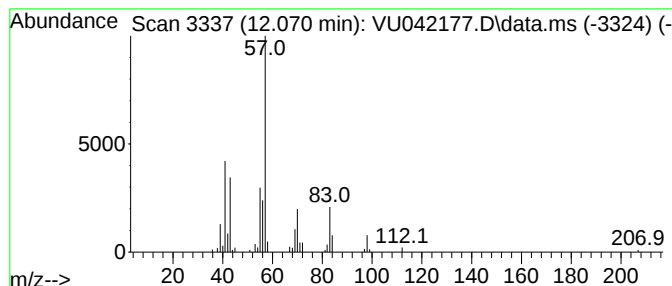
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	1.28 ug/L	82803	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-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53



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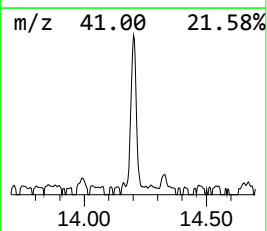
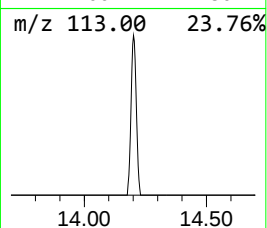
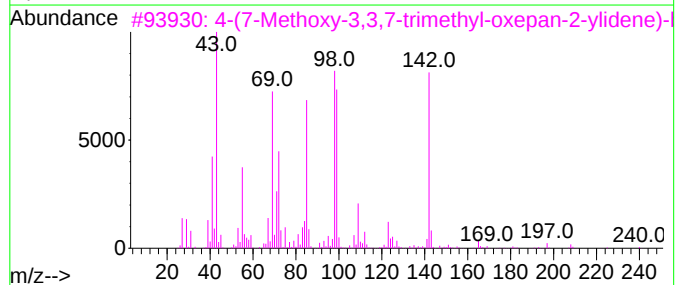
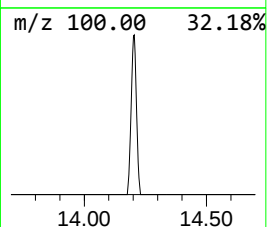
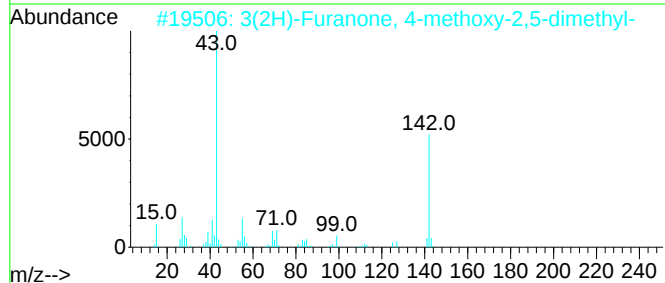
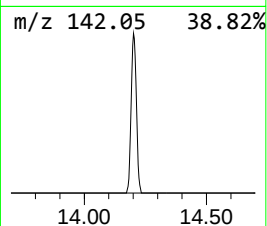
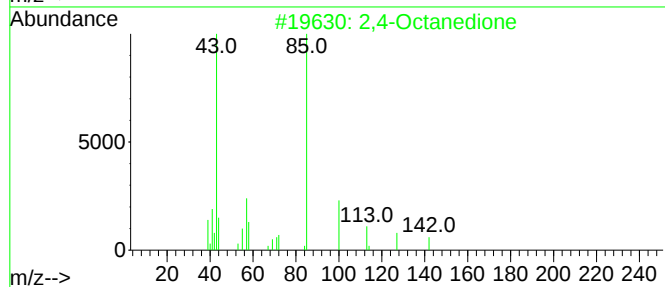
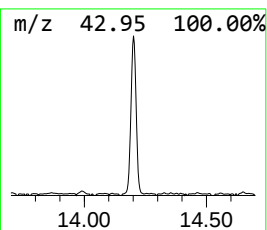
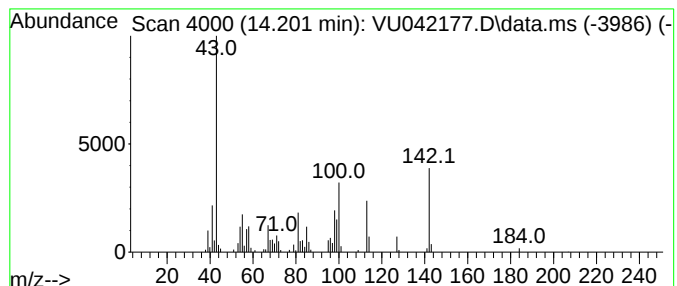
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Peak Number 5 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	1.35 ug/L	87805	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	43
3			4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	25
4			Isoxazole, 3,5-dimethyl-4-nitro-	142	C5H6N2O3	001123-49-5	22
5			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	12



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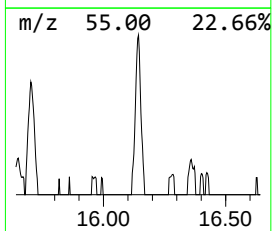
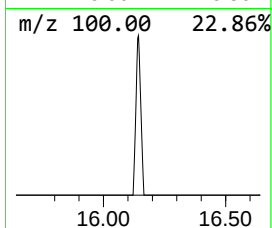
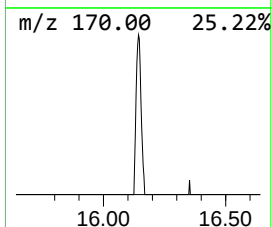
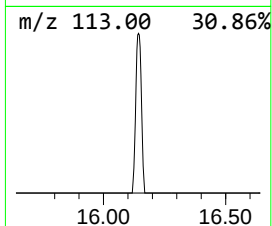
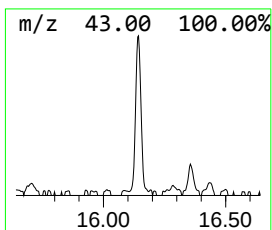
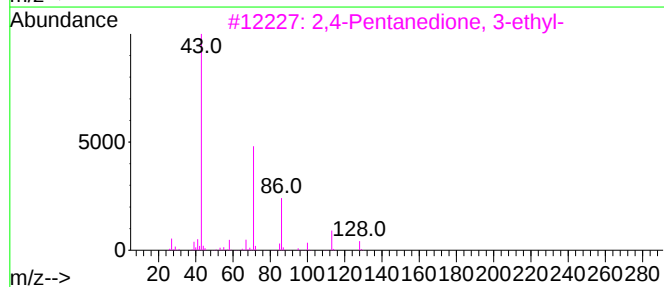
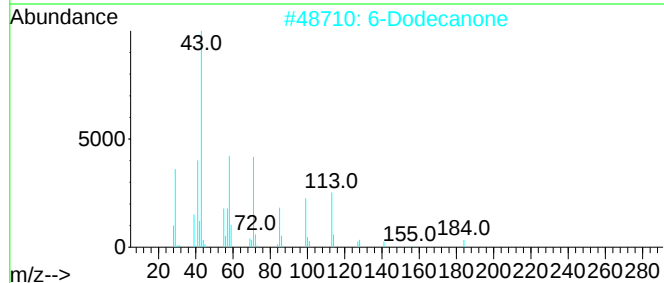
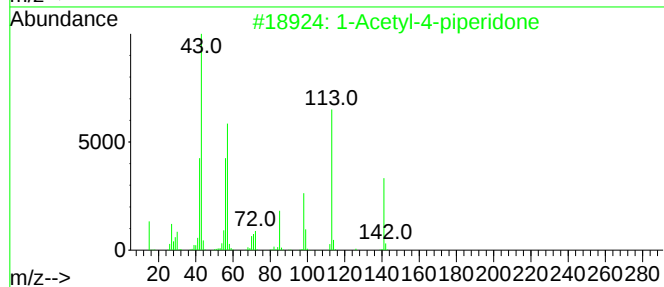
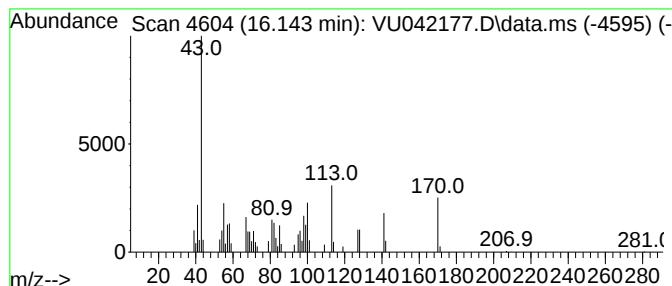
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
16.143	0.53 ug/L	34579	1,4-Dichlorobenzene-d4		11.819	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1-Acetyl-4-piperidone		141	C7H11NO2	032161-06-1	16
2	6-Dodecanone		184	C12H24O	006064-27-3	16
3	2,4-Pentanedione, 3-ethyl-		128	C7H12O2	001540-34-7	14
4	2,4-Octanedione		142	C8H14O2	014090-87-0	14
5	Pyrrolidine, 1-(1-oxobutyl)-		141	C8H15NO	033527-93-4	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042177.D
Acq On : 22 Jan 2021 18:10
Operator : SY/MD
Sample : M1222-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

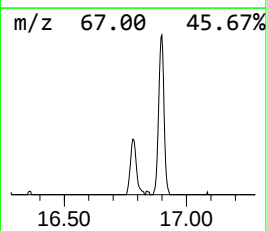
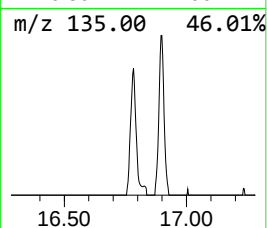
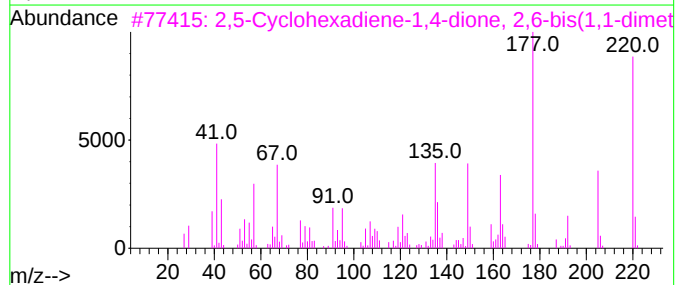
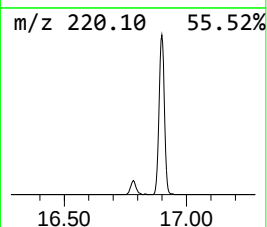
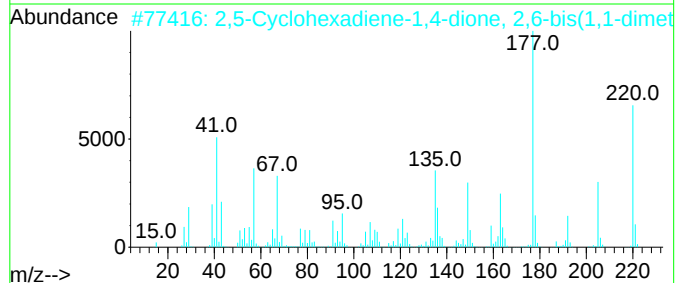
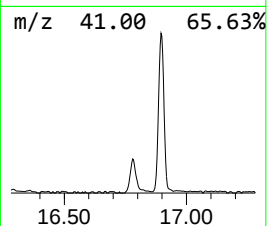
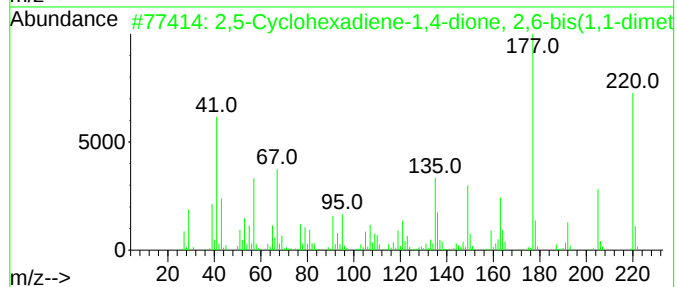
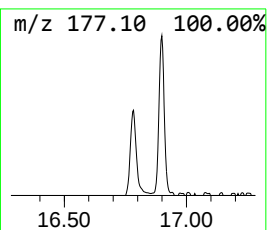
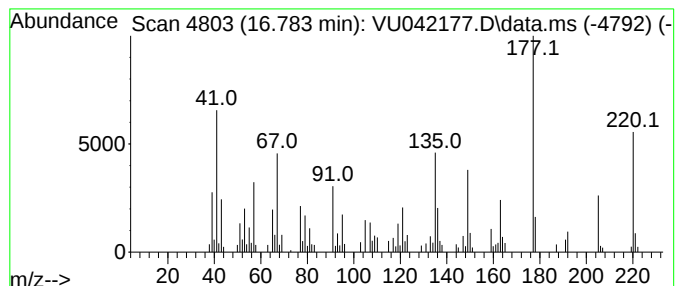
Instrument :
MSVOA_D
ClientSampleId :

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.783	1.21 ug/L	78264	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	94
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	70
4	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	55
5	2H-1-Benzopyran, 3,5,6,8a-tetra...	192	C13H20O	041678-29-9	51



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042177.D
Acq On : 22 Jan 2021 18:10
Operator : SY/MD
Sample : M1222-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :

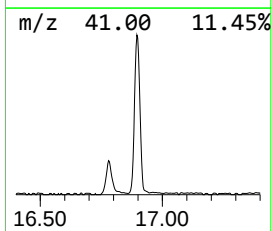
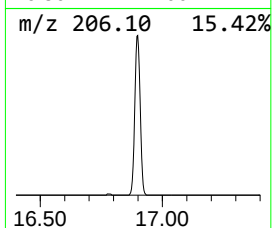
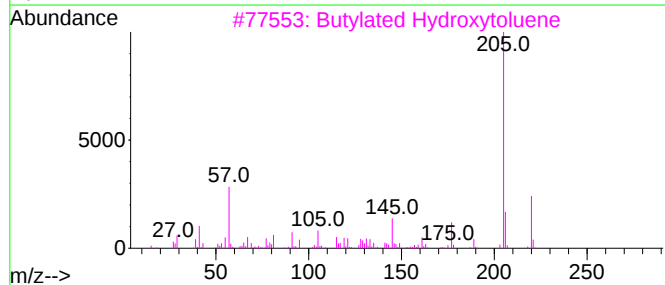
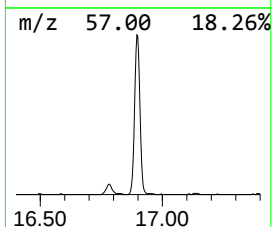
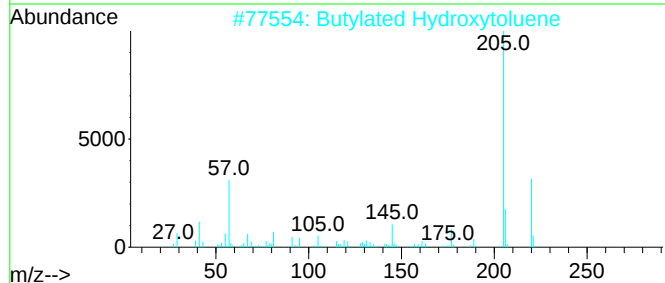
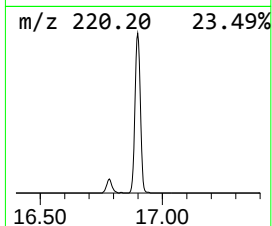
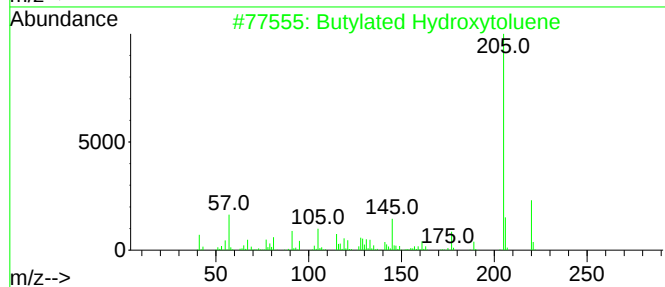
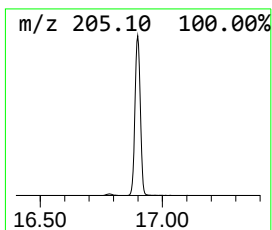
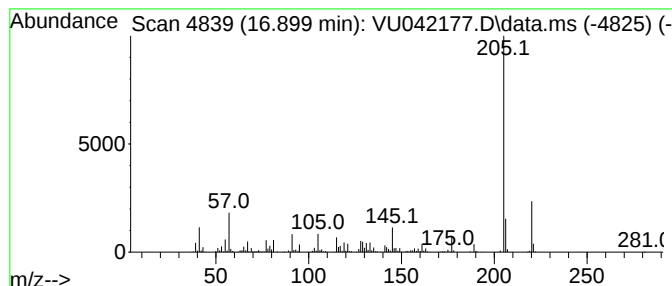
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	10.71 ug/L	695208	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	95
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5			Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
Data File : VU042177.D
Acq On : 22 Jan 2021 18:10
Operator : SY/MD
Sample : M1222-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 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...	7.185	1.5	ug/L	74974	1	6.256	245604	5.0
Cyclopentene, 1...	9.648	0.5	ug/L	31342	2	9.423	309731	5.0
1-Hexanol, 2-et...	12.070	1.3	ug/L	82803	3	11.819	324546	5.0
unknown-01	14.201	1.4	ug/L	87805	3	11.819	324546	5.0
unknown-02	16.143	0.5	ug/L	34579	3	11.819	324546	5.0
2,5-Cyclohexadi...	16.783	1.2	ug/L	78264	3	11.819	324546	5.0
Butylated Hydro...	16.899	10.7	ug/L	695208	3	11.819	324546	5.0