

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042169.D
 Acq On : 22 Jan 2021 14:57
 Operator : SY/MD
 Sample : M1222-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 9 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: VU042169.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	14	rVB2	20105	17004	3.93%	0.435%
2	1.591	67	78	87	rVB2	45986	68823	15.89%	1.762%
3	1.726	114	120	129	rBV4	3449	4568	1.05%	0.117%
4	1.909	169	177	193	rVB	33157	43398	10.02%	1.111%
5	2.562	369	380	394	rBV	67219	105614	24.38%	2.704%
6	4.729	1019	1054	1083	rBV2	31029	154853	35.75%	3.965%
7	5.070	1142	1160	1181	rVB2	70773	159715	36.87%	4.089%
8	5.729	1343	1365	1391	rBV2	147173	358156	82.68%	9.170%
9	6.256	1514	1529	1549	rVB	116076	213323	49.25%	5.462%
10	6.645	1640	1650	1655	rBV4	5114	8794	2.03%	0.225%
11	6.700	1655	1667	1690	rVB	87254	171257	39.53%	4.385%
12	7.186	1800	1818	1834	rBV	28724	59201	13.67%	1.516%
13	7.571	1927	1938	1957	rVB	51127	88677	20.47%	2.270%
14	7.903	2029	2041	2055	rVB	167723	284123	65.59%	7.274%
15	7.977	2055	2064	2073	rVB2	4561	7510	1.73%	0.192%
16	8.050	2078	2087	2096	rVB3	3150	5744	1.33%	0.147%
17	8.189	2119	2130	2143	rBV	32749	55408	12.79%	1.419%
18	8.501	2217	2227	2237	rVB2	4839	8604	1.99%	0.220%
19	8.559	2237	2245	2254	rVB5	5161	7771	1.79%	0.199%
20	8.652	2260	2274	2288	rBV	221878	410642	94.80%	10.514%
21	9.423	2502	2514	2534	rBV	158935	264117	60.97%	6.762%
22	9.649	2577	2584	2594	rVB	10771	15323	3.54%	0.392%
23	9.774	2612	2623	2638	rVB4	2657	5387	1.24%	0.138%
24	10.693	2901	2909	2920	rVB3	8512	13223	3.05%	0.339%
25	10.764	2920	2931	2943	rBV	68872	110434	25.49%	2.827%
26	10.899	2967	2973	2984	rVB5	3116	4530	1.05%	0.116%
27	10.973	2987	2996	3012	rVB	11686	19084	4.41%	0.489%
28	11.819	3247	3259	3274	rVB	175554	275930	63.70%	7.065%
29	11.899	3274	3284	3294	rBV4	4300	7014	1.62%	0.180%
30	11.986	3303	3311	3327	rVB7	2687	5162	1.19%	0.132%
31	12.073	3327	3338	3344	rBV5	4690	8798	2.03%	0.225%
32	12.201	3366	3378	3391	rBV	174689	280353	64.72%	7.178%
33	12.330	3408	3418	3431	rBV2	18233	27892	6.44%	0.714%
34	12.780	3551	3558	3568	rVB5	3714	5224	1.21%	0.134%
35	12.896	3582	3594	3603	rBV2	9444	14478	3.34%	0.371%
36	12.954	3603	3612	3621	rVV6	4030	6138	1.42%	0.157%

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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

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 Title : TRACE VOA SOM01.0

37	13.012	3624	3630	3643	rVB4	2923	4615	1.07%	0.118%
38	14.201	3985	4000	4016	rBV	40450	60788	14.03%	1.556%
39	14.327	4029	4039	4048	rBV3	6334	9608	2.22%	0.246%
40	15.008	4243	4251	4262	rVB7	3174	5905	1.36%	0.151%
41	15.703	4456	4467	4480	rBV6	16862	26446	6.10%	0.677%
42	16.143	4596	4604	4612	rVB5	8390	11770	2.72%	0.301%
43	16.783	4794	4803	4813	rBV2	37893	57218	13.21%	1.465%
44	16.899	4828	4839	4857	rBV	294022	433187	100.00%	11.091%

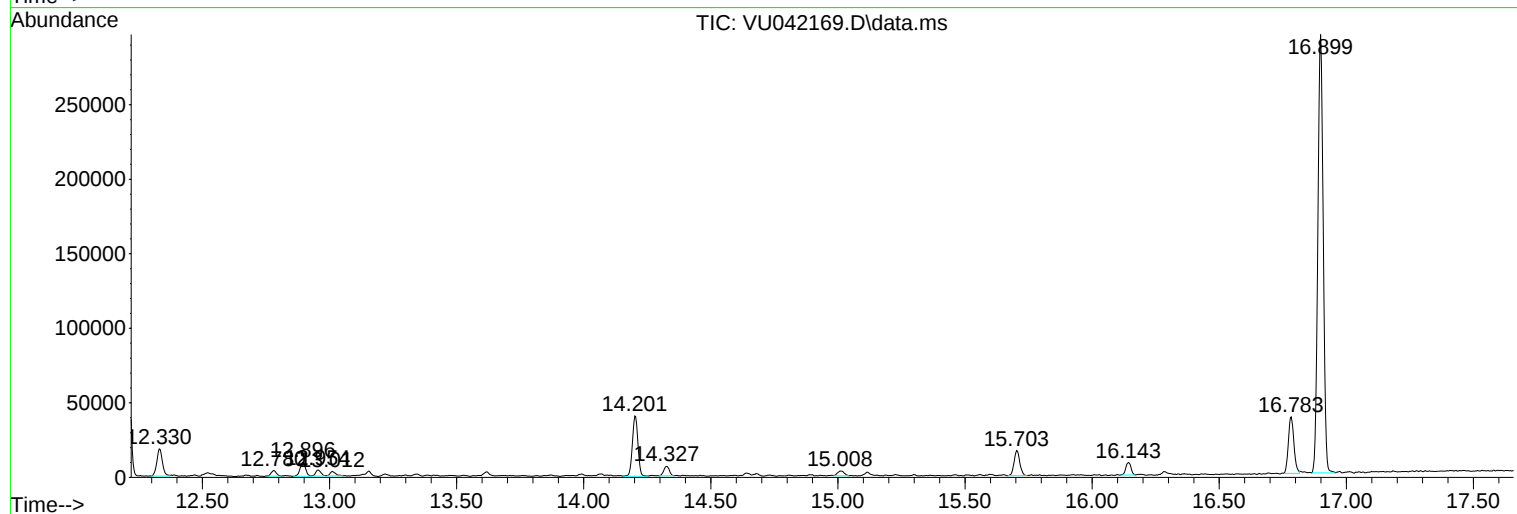
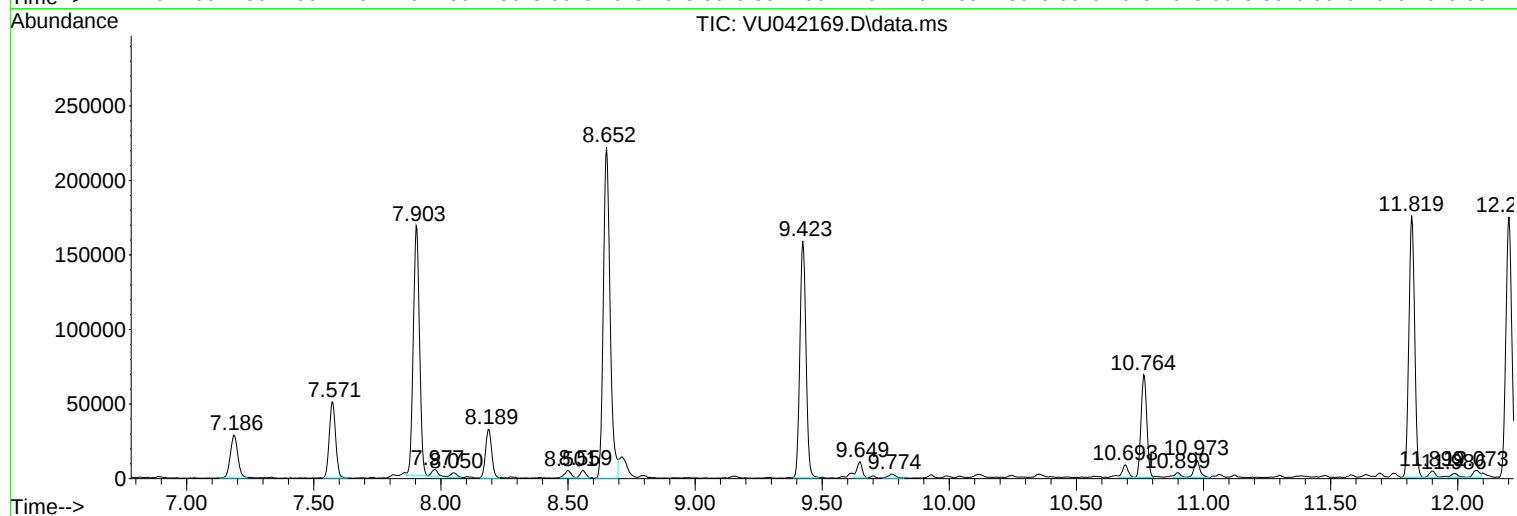
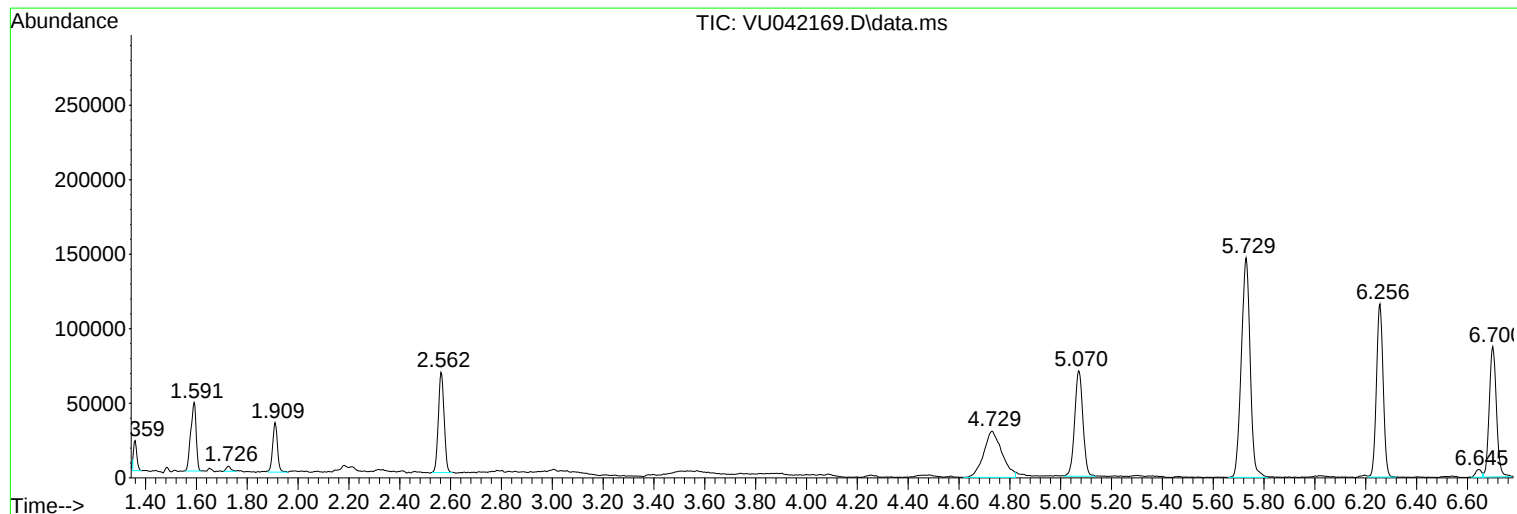
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Instrument :
MSVOA_D
ClientSampleId :

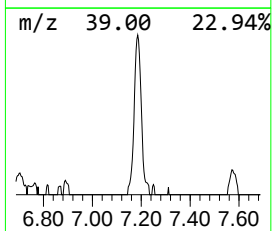
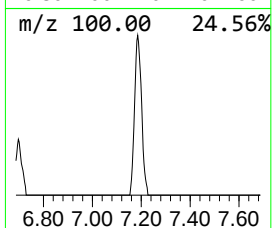
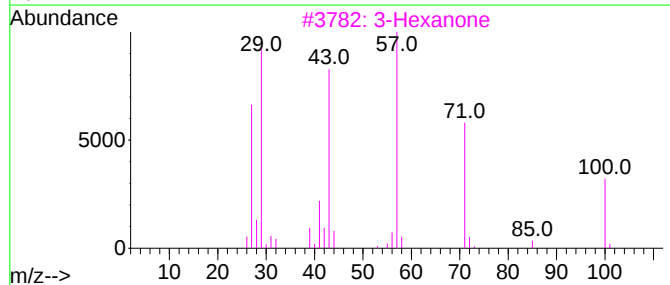
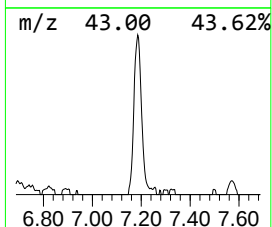
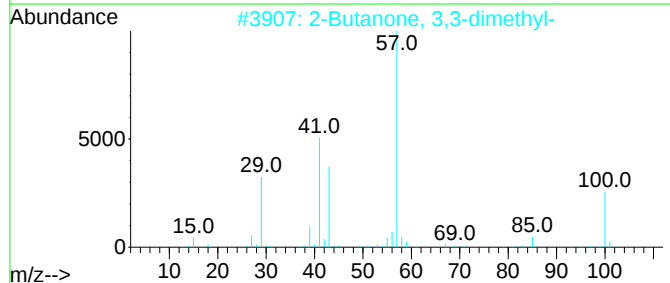
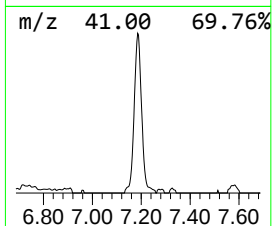
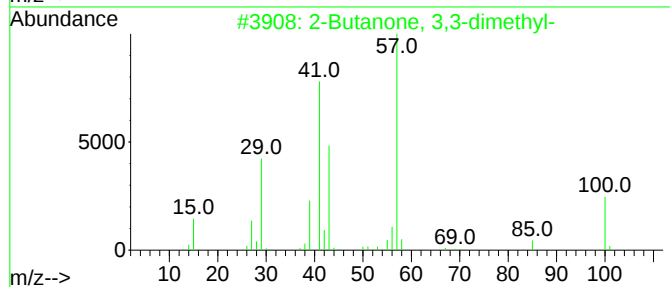
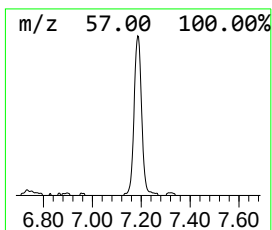
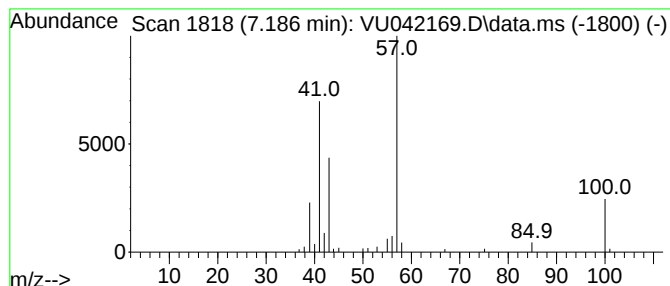
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.186	1.39 ug/L	59201	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	91	
2	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	83	
3	3-Hexanone	100	C6H12O	000589-38-8	50	
4	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	50	
5	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	47	



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Instrument :
MSVOA_D
ClientSampleId :

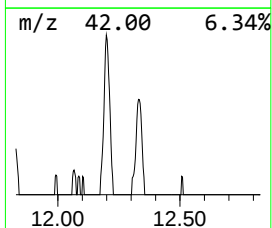
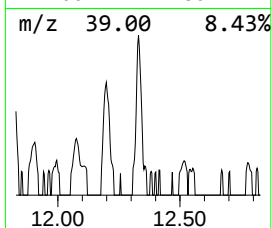
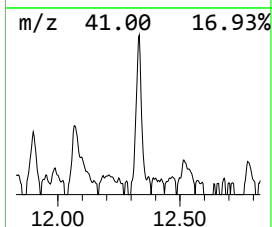
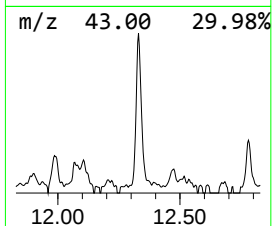
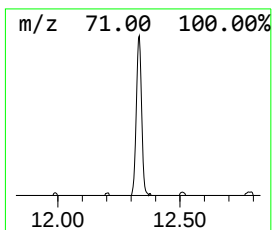
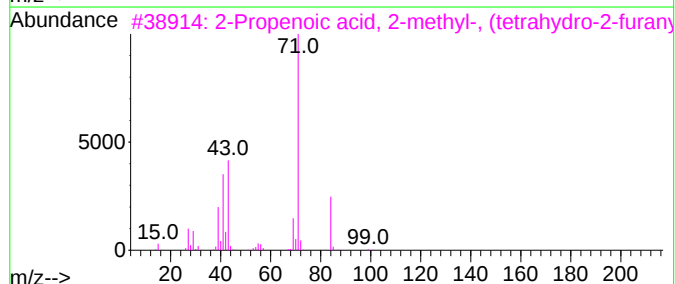
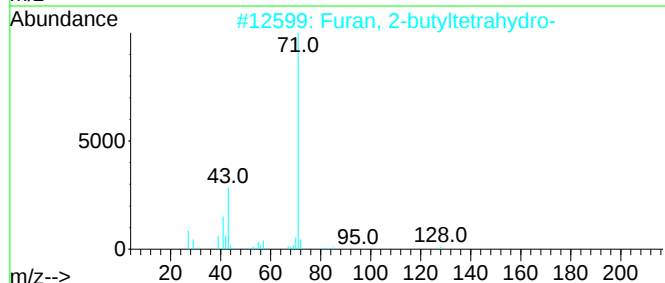
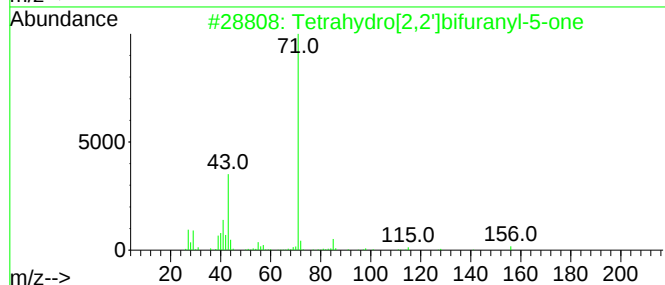
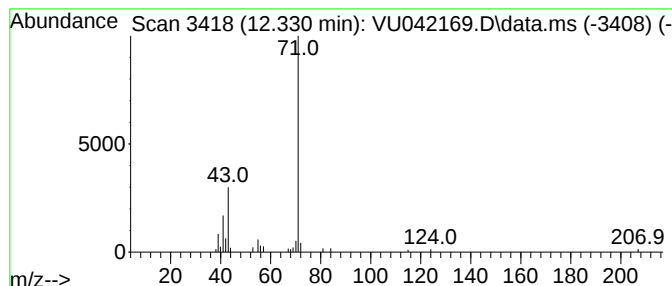
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Tetrahydro[2,2']bifuranyl-5... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	0.51 ug/L	27892	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrahydro[2,2']bifuranyl-5-one	156	C8H12O3	019680-00-3	72
2			Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	72
3			2-Propenoic acid, 2-methyl-, (te...	170	C9H14O3	002455-24-5	72
4			Tetrahydrofuran, 2-propyl-	114	C7H14O	003208-22-8	72
5			Glutaric acid, ditetrahydrofurfu...	300	C15H24O6	1000359-67-4	56



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ALS Vial : 9 Sample Multiplier: 1

Instrument :
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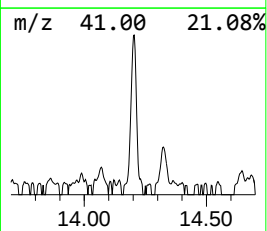
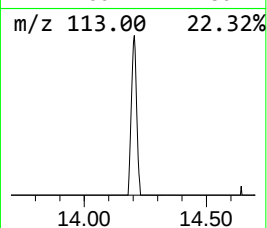
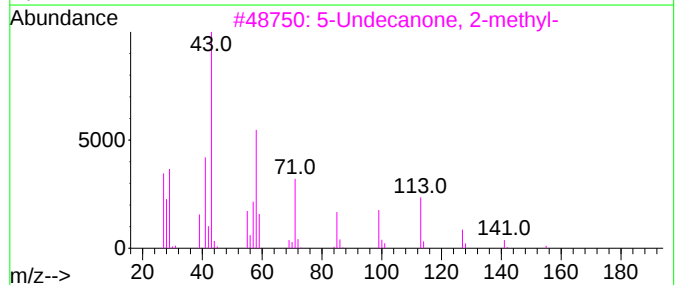
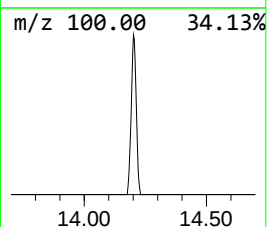
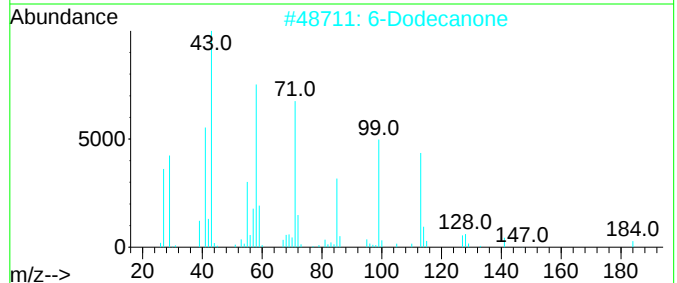
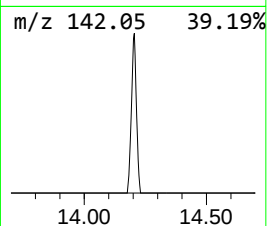
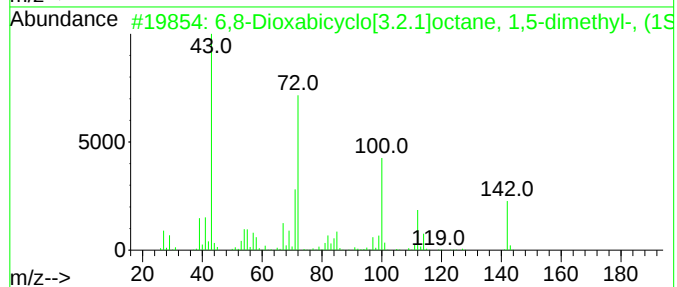
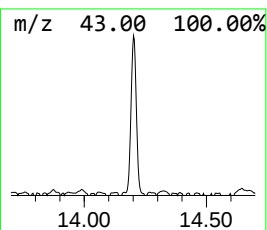
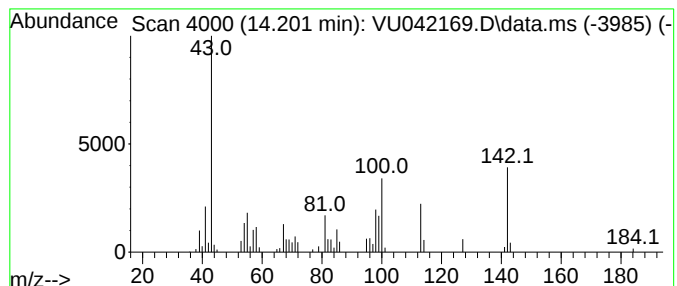
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	1.10 ug/L	60788	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	25		
2	6-Dodecanone	184	C12H24O	006064-27-3	12		
3	5-Undecanone, 2-methyl-	184	C12H24O	050639-02-6	12		
4	Hexanoic Acid, 2,2,2-trifluoroet...	198	C8H13F3O2	1000376-58-3	12		
5	6-Dodecanone	184	C12H24O	006064-27-3	10		



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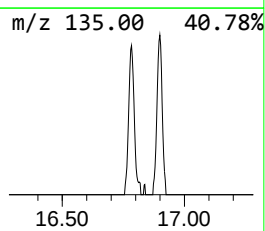
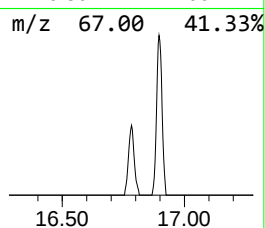
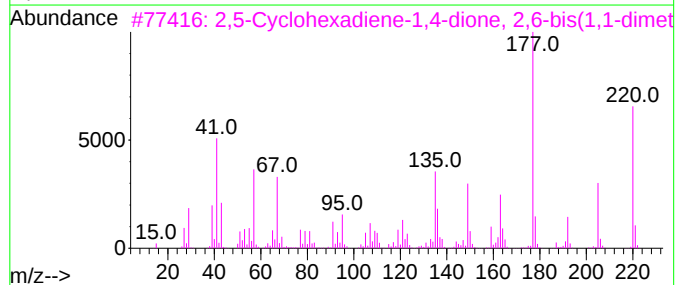
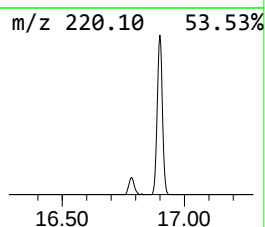
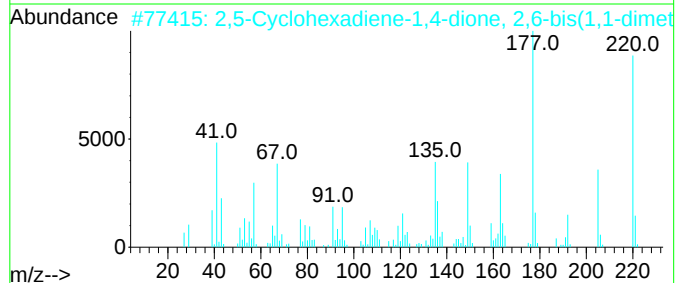
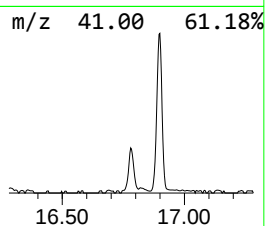
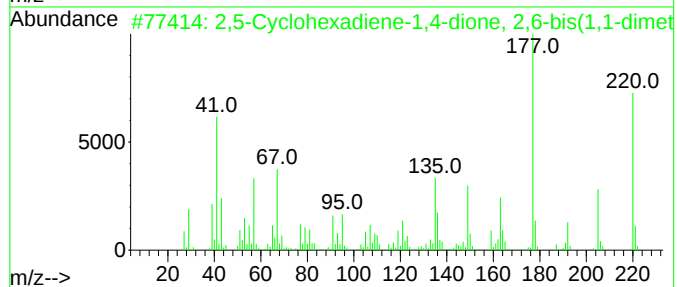
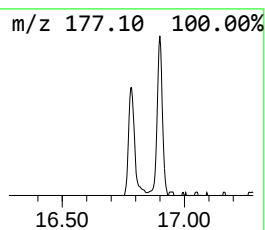
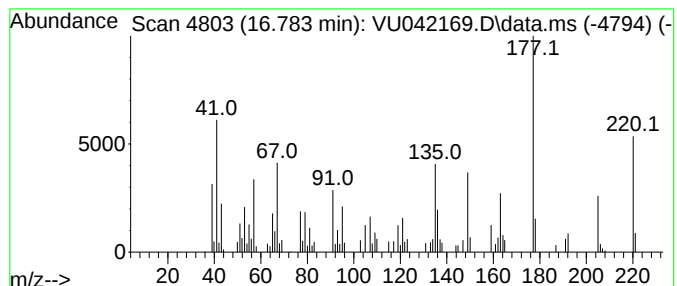
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.783	1.04 ug/L	57218	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	97
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	93
4			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	30
5			trans-.beta.-Ionone	192	C13H20O	000079-77-6	30



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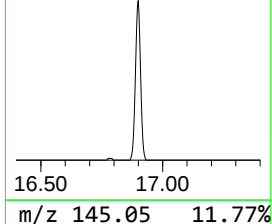
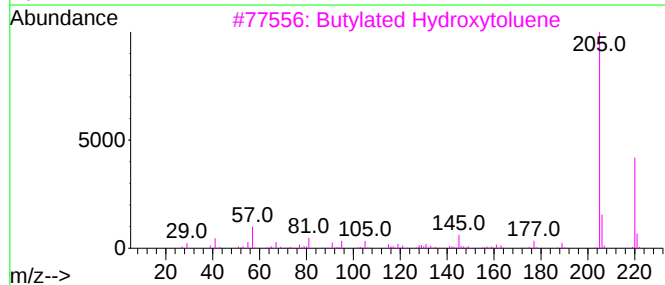
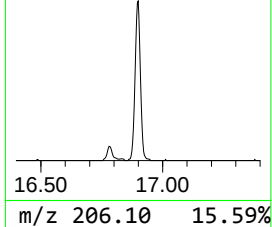
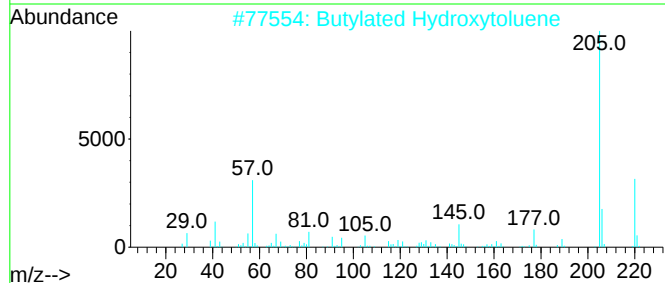
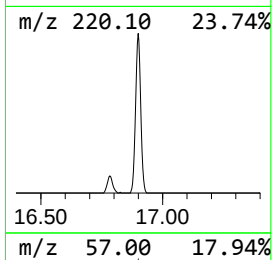
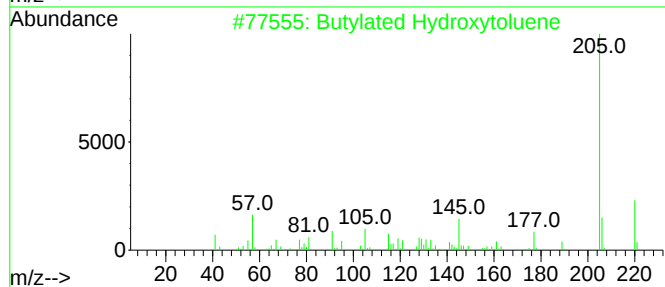
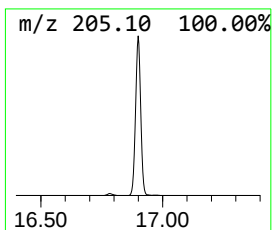
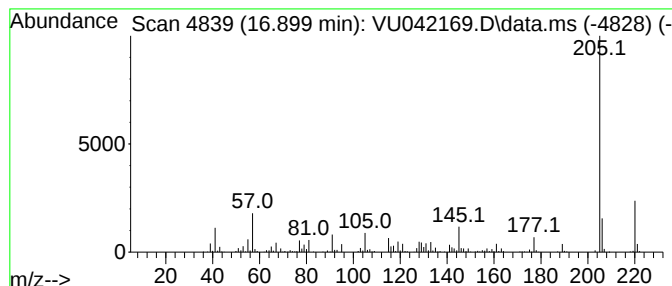
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	7.85 ug/L	433187	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 : VU042169.D
Acq On : 22 Jan 2021 14:57
Operator : SY/MD
Sample : M1222-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 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...	7.186	1.4	ug/L	59201	1	6.256	213323	5.0
Tetrahydro[2,2'...	12.330	0.5	ug/L	27892	3	11.819	275930	5.0
unknown-01	14.201	1.1	ug/L	60788	3	11.819	275930	5.0
2,5-Cyclohexadi...	16.783	1.0	ug/L	57218	3	11.819	275930	5.0
Butylated Hydro...	16.899	7.8	ug/L	433187	3	11.819	275930	5.0