

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042175.D
 Acq On : 22 Jan 2021 17:22
 Operator : SY/MD
 Sample : M1222-10
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 F1E17

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: VU042175.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	25	rVB2	12067	14384	3.24%	0.353%
2	1.600	69	81	90	rVB2	49540	72028	16.24%	1.770%
3	1.916	171	179	191	rVB	35180	45878	10.34%	1.127%
4	2.571	372	383	396	rBV	75833	122782	27.68%	3.017%
5	3.250	571	594	596	rBV3	9581	24181	5.45%	0.594%
6	4.652	1011	1030	1061	rBV3	43992	178623	40.28%	4.389%
7	5.073	1146	1161	1179	rBV	70449	153243	34.55%	3.766%
8	5.732	1345	1366	1384	rBV3	135876	357181	80.54%	8.777%
9	6.256	1515	1529	1547	rBV	130318	244381	55.10%	6.005%
10	6.549	1609	1620	1631	rVB5	6694	12254	2.76%	0.301%
11	6.700	1653	1667	1684	rVB	87934	168763	38.05%	4.147%
12	7.176	1797	1815	1839	rBV2	27971	57336	12.93%	1.409%
13	7.574	1924	1939	1952	rBV	49590	88887	20.04%	2.184%
14	7.832	1999	2019	2029	rBV4	8578	20765	4.68%	0.510%
15	7.906	2029	2042	2057	rVV	172318	296354	66.82%	7.282%
16	7.976	2058	2064	2073	rVV4	2826	5902	1.33%	0.145%
17	8.041	2076	2084	2097	rVB4	3483	6592	1.49%	0.162%
18	8.185	2119	2129	2142	rBV	32239	54944	12.39%	1.350%
19	8.494	2214	2225	2235	rBV3	3652	6386	1.44%	0.157%
20	8.562	2235	2246	2257	rVB	45841	77173	17.40%	1.896%
21	8.642	2257	2271	2294	rBV	213168	427343	96.36%	10.501%
22	9.423	2502	2514	2537	rBV	182262	306860	69.19%	7.540%
23	9.648	2577	2584	2594	rVB	7246	10671	2.41%	0.262%
24	9.771	2612	2622	2629	rBV4	3491	6109	1.38%	0.150%
25	10.111	2720	2728	2741	rVB8	2475	4677	1.05%	0.115%
26	10.693	2901	2909	2918	rVB3	5038	8092	1.82%	0.199%
27	10.764	2919	2931	2950	rBV	68611	111989	25.25%	2.752%
28	10.973	2984	2996	3007	rVV2	4709	8488	1.91%	0.209%
29	11.819	3248	3259	3276	rVB	203969	327387	73.82%	8.045%
30	12.069	3329	3337	3361	rBV2	7184	15844	3.57%	0.389%
31	12.201	3366	3378	3395	rVB	181237	291424	65.71%	7.161%
32	12.333	3407	3419	3432	rBV	6673	10237	2.31%	0.252%
33	12.896	3585	3594	3603	rBV5	5224	7607	1.72%	0.187%
34	14.201	3991	4000	4013	rBV2	29282	43285	9.76%	1.064%
35	15.703	4460	4467	4477	rVB5	3880	5899	1.33%	0.145%
36	16.143	4593	4604	4616	rBV6	7722	11078	2.50%	0.272%

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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	16.780	4794	4802	4813	rBV5	13447	21098	4.76%	0.518%
38	16.899	4828	4839	4853	rBV	304416	443502	100.00%	10.898%

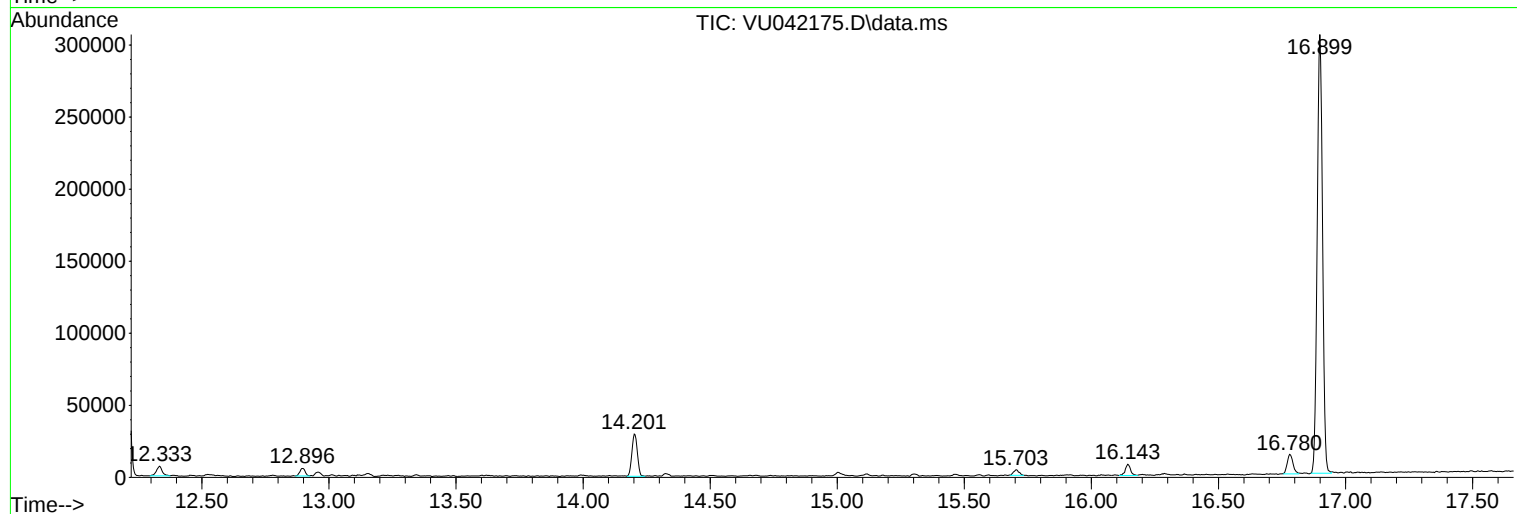
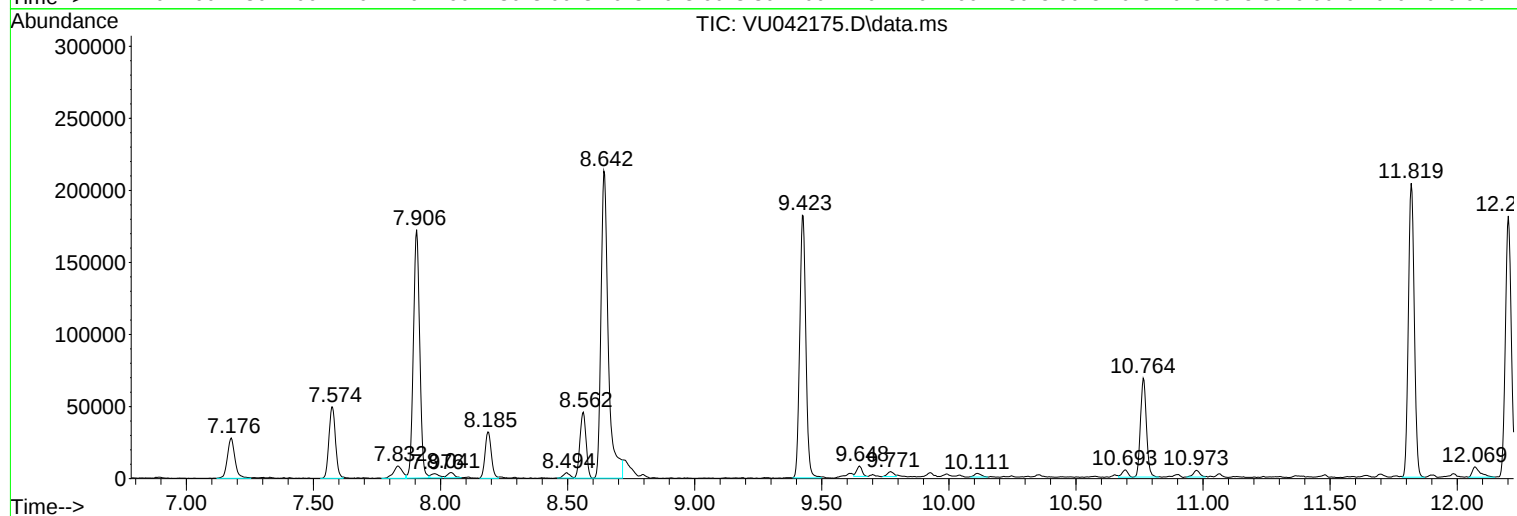
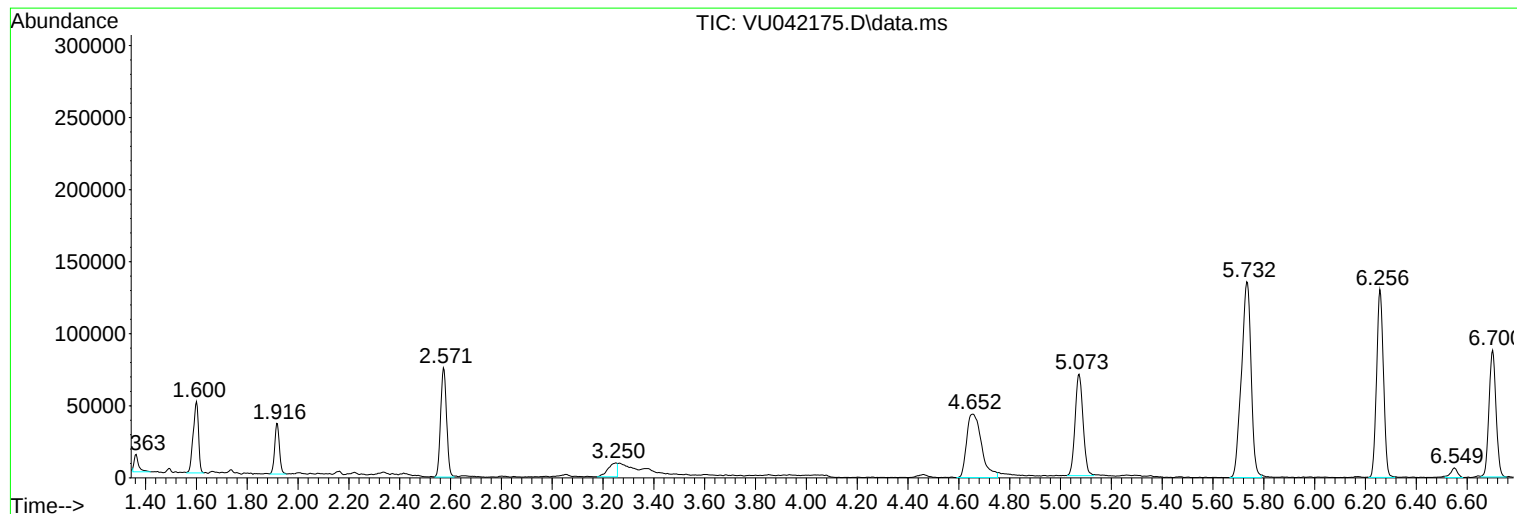
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
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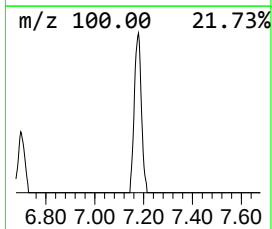
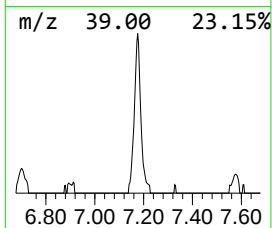
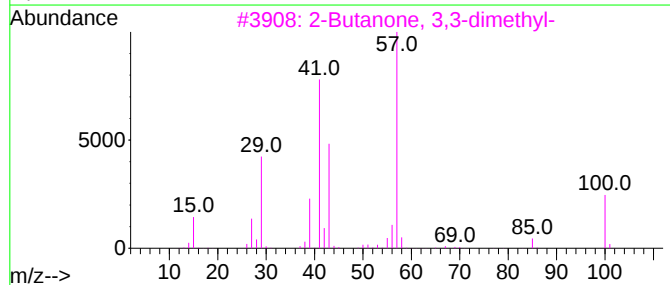
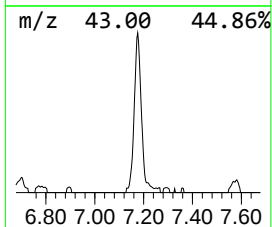
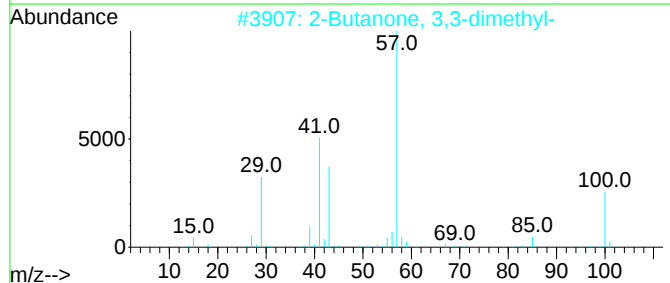
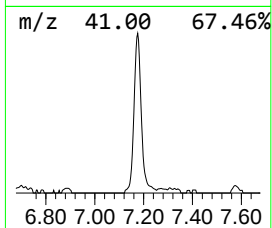
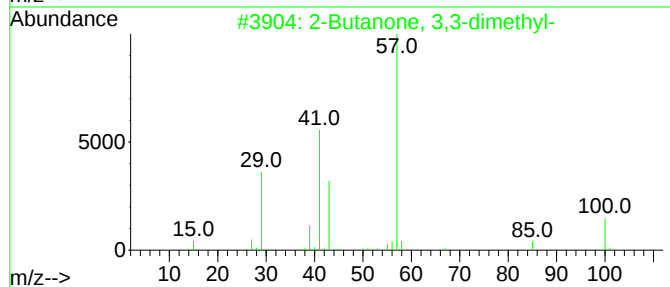
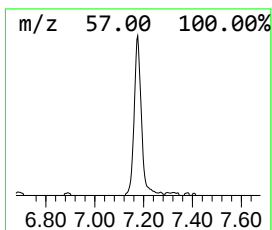
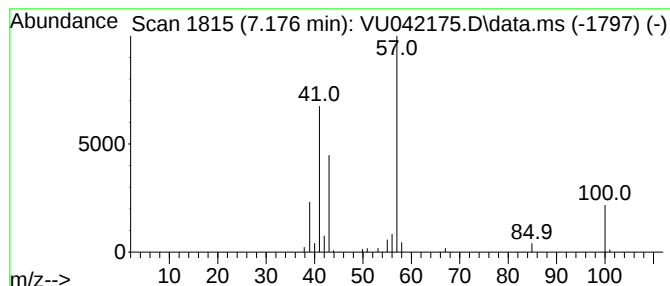
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.176	1.17 ug/L	57336	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	90
3	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	83
4	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	72
5	3-Hexanone			100	C6H12O	000589-38-8	53



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
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ClientSampleId :
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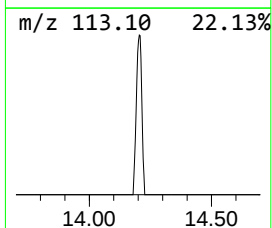
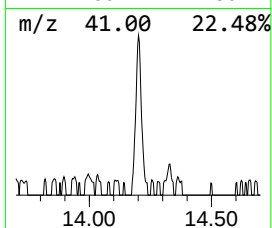
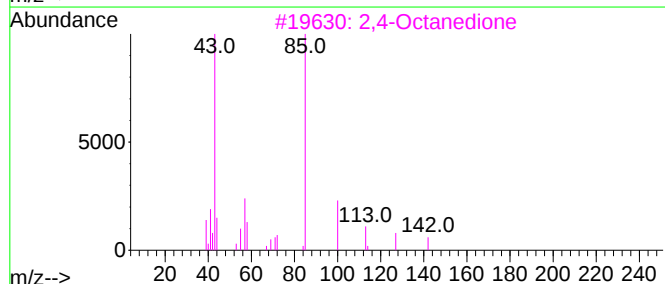
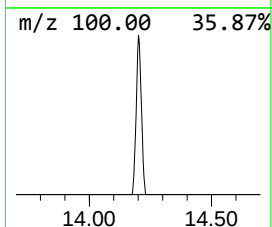
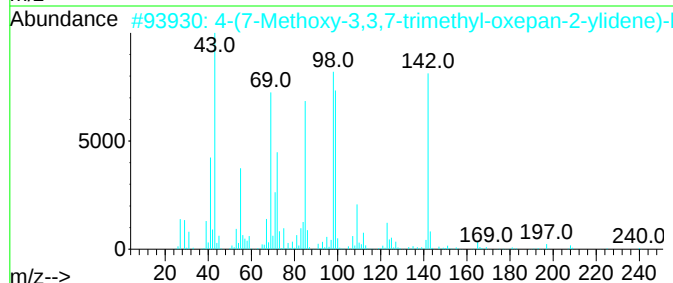
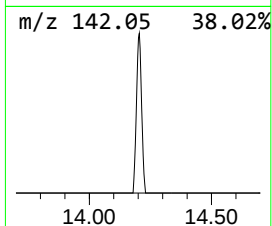
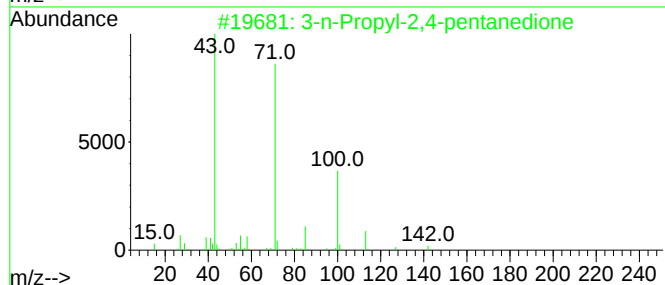
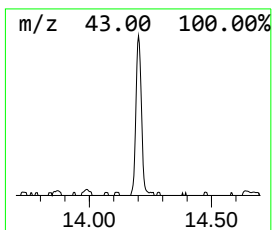
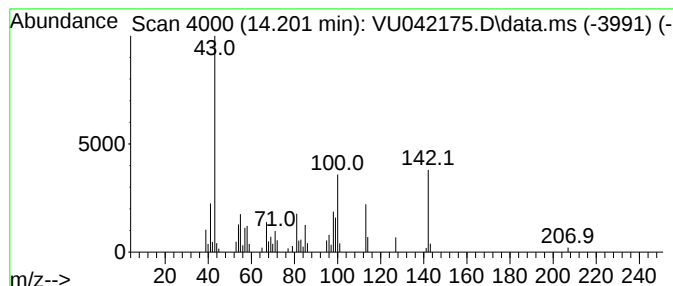
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	0.66 ug/L	43285	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-n-Propyl-2,4-pentanedione	142	C8H14O2	001540-35-8	38
2			4-(7-Methoxy-3,3,7-trimethyl-oxe...	240	C14H24O3	107675-07-0	38
3			2,4-Octanedione	142	C8H14O2	014090-87-0	32
4			6-Dodecanone	184	C12H24O	006064-27-3	25
5			6-Dodecanone	184	C12H24O	006064-27-3	25



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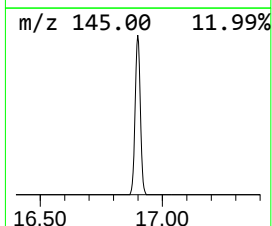
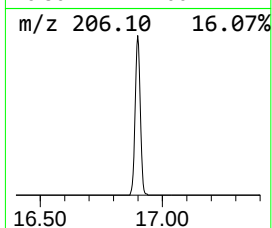
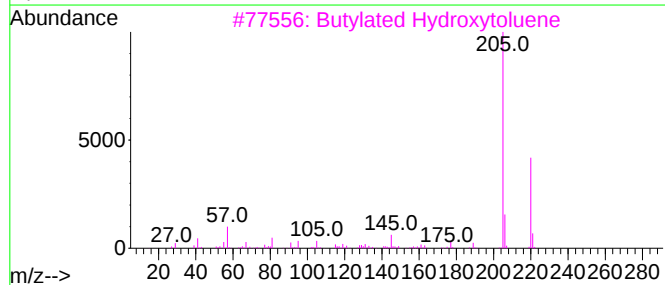
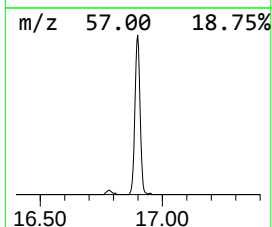
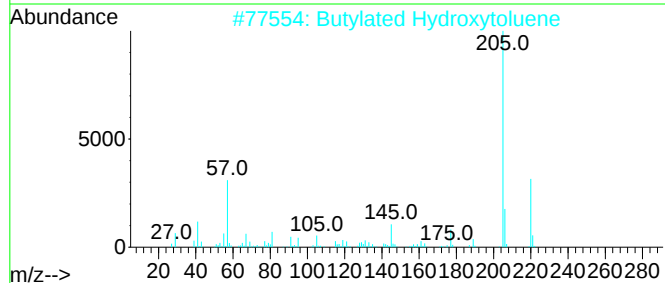
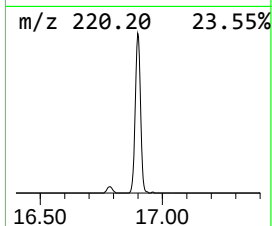
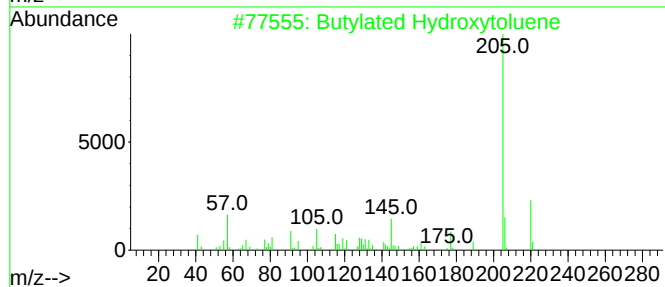
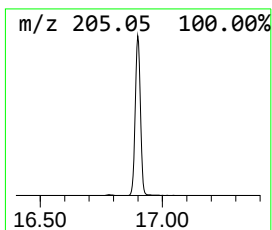
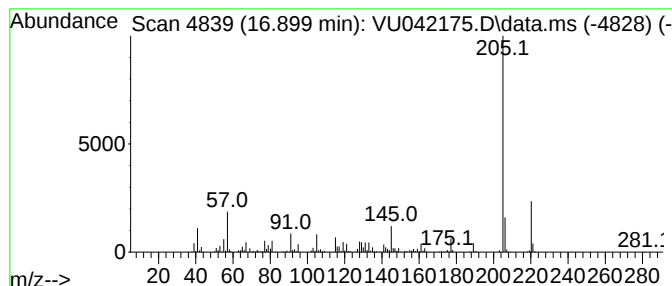
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	6.77 ug/L	443502	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
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



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanone, 3,3...	7.176	1.2	ug/L	57336	1	6.256	244381	5.0
unknown-01	14.201	0.7	ug/L	43285	3	11.819	327387	5.0
Butylated Hydro...	16.899	6.8	ug/L	443502	3	11.819	327387	5.0