

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042171.D
 Acq On : 22 Jan 2021 15:45
 Operator : SY/MD
 Sample : M1222-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 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: VU042171.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	18	rVB2	10682	11646	1.81%	0.284%
2	1.600	70	81	89	rVB2	45195	59873	9.33%	1.458%
3	1.916	167	179	188	rBV	34631	44748	6.97%	1.090%
4	2.572	372	383	398	rBV	75725	122096	19.02%	2.974%
5	3.266	578	599	605	rBV3	5158	17523	2.73%	0.427%
6	4.649	1013	1029	1056	rBV	39154	129079	20.11%	3.144%
7	5.073	1146	1161	1178	rBV	71055	151753	23.64%	3.696%
8	5.732	1346	1366	1393	rBV2	133519	354663	55.26%	8.638%
9	6.256	1516	1529	1549	rBV	129474	241478	37.62%	5.881%
10	6.700	1653	1667	1684	rVB	87457	168199	26.21%	4.096%
11	7.176	1795	1815	1834	rBV2	26333	56107	8.74%	1.366%
12	7.575	1926	1939	1955	rBV	50416	89916	14.01%	2.190%
13	7.829	1999	2018	2030	rBV8	4944	16469	2.57%	0.401%
14	7.906	2030	2042	2057	rVV	167175	293045	45.66%	7.137%
15	7.980	2057	2065	2075	rVV4	4890	10198	1.59%	0.248%
16	8.038	2078	2083	2096	rVB4	3671	6653	1.04%	0.162%
17	8.185	2119	2129	2147	rBV	31814	53956	8.41%	1.314%
18	8.642	2259	2271	2285	rBV	207143	395560	61.63%	9.634%
19	9.423	2502	2514	2533	rBV	177792	303066	47.22%	7.381%
20	9.648	2577	2584	2594	rVB2	11633	17464	2.72%	0.425%
21	9.771	2612	2622	2640	rVB4	3343	7320	1.14%	0.178%
22	10.243	2761	2769	2782	rBV2	6291	10855	1.69%	0.264%
23	10.693	2899	2909	2920	rVB3	9788	15828	2.47%	0.385%
24	10.764	2920	2931	2949	rBV	67801	113095	17.62%	2.754%
25	10.973	2982	2996	3011	rVB	13422	24674	3.84%	0.601%
26	11.819	3247	3259	3275	rVB	198721	316906	49.38%	7.718%
27	11.899	3275	3284	3295	rBV2	4874	7424	1.16%	0.181%
28	12.073	3327	3338	3345	rBV2	11786	21118	3.29%	0.514%
29	12.201	3365	3378	3391	rVB	178224	286956	44.71%	6.989%
30	12.330	3403	3418	3435	rBV	20659	35346	5.51%	0.861%
31	12.896	3583	3594	3603	rBV5	4810	7256	1.13%	0.177%
32	14.201	3987	4000	4009	rBV2	25602	38276	5.96%	0.932%
33	14.327	4028	4039	4048	rVB3	4561	6875	1.07%	0.167%
34	15.706	4457	4468	4478	rBV8	10331	16683	2.60%	0.406%
35	16.783	4795	4803	4814	rBV7	7628	12100	1.89%	0.295%
36	16.899	4825	4839	4855	rBV	433302	641819	100.00%	15.631%

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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

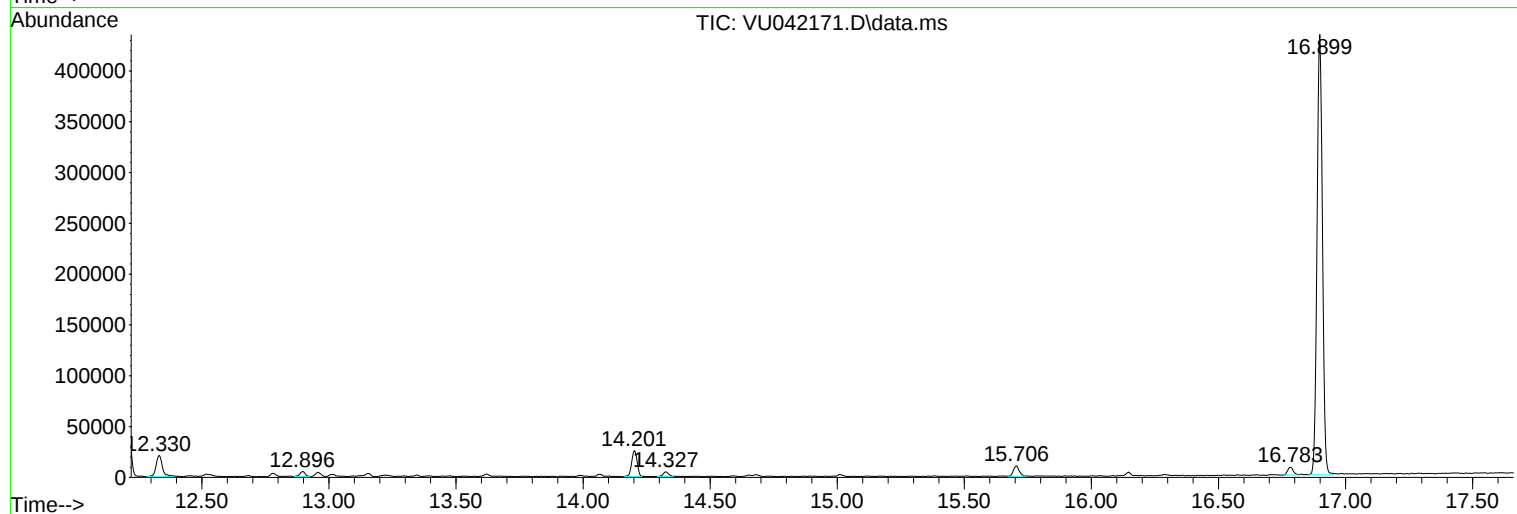
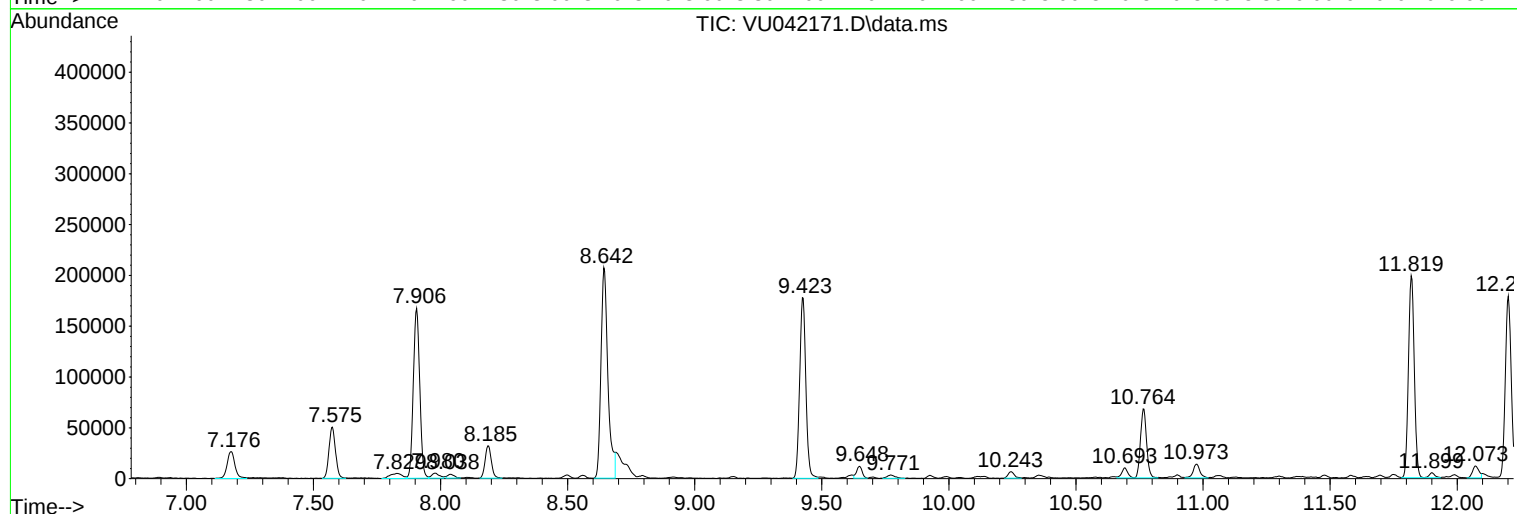
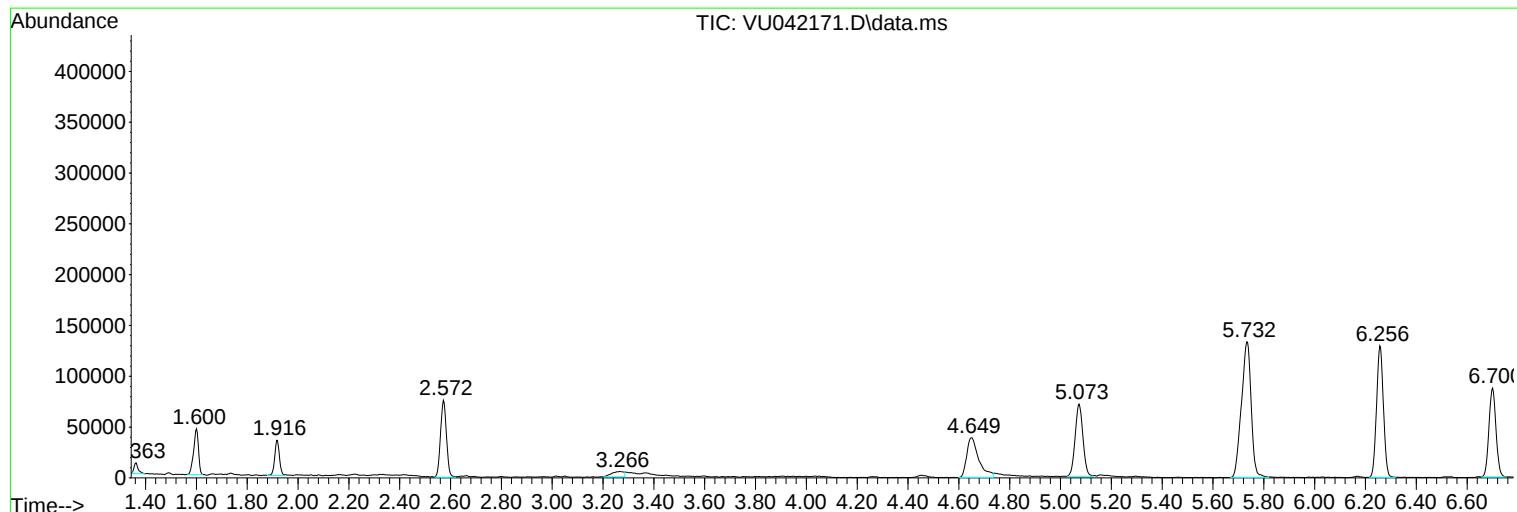
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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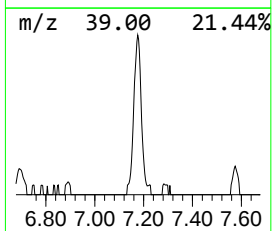
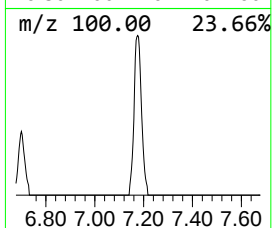
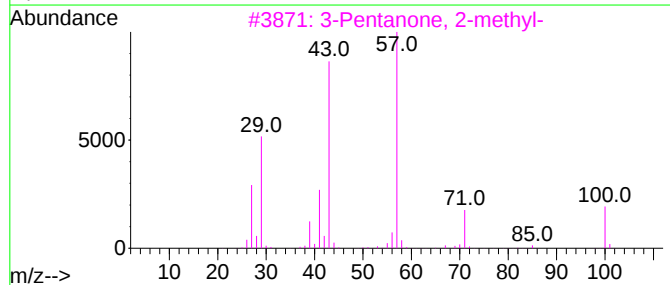
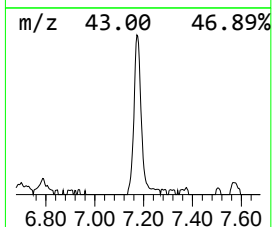
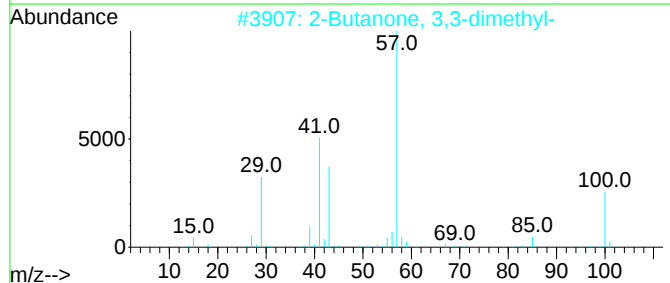
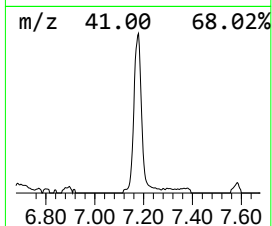
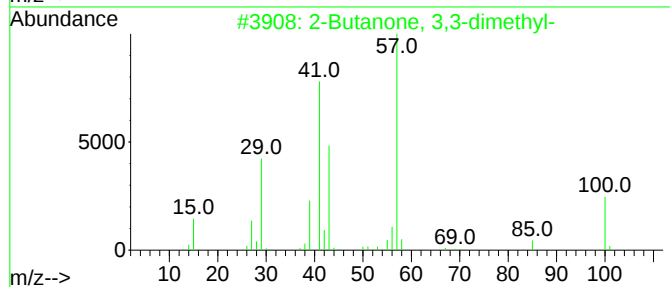
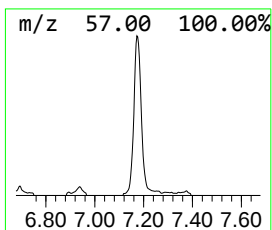
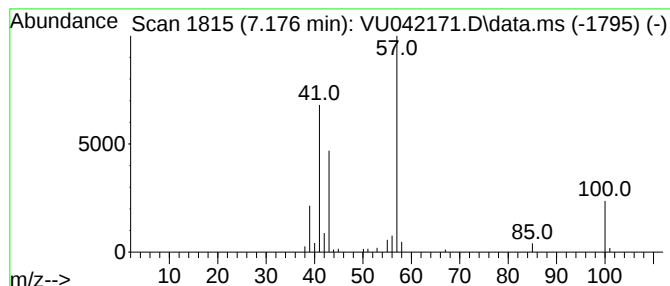
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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	1.16 ug/L	56107	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	80
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	64
4	3-Hexanone			100	C6H12O	000589-38-8	53
5	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	53



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Instrument :
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ClientSampleId :

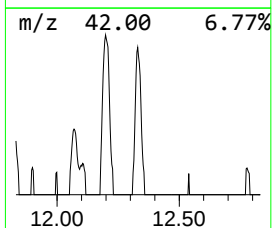
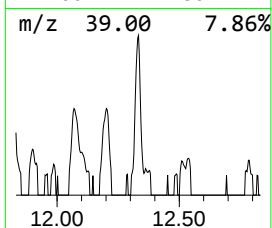
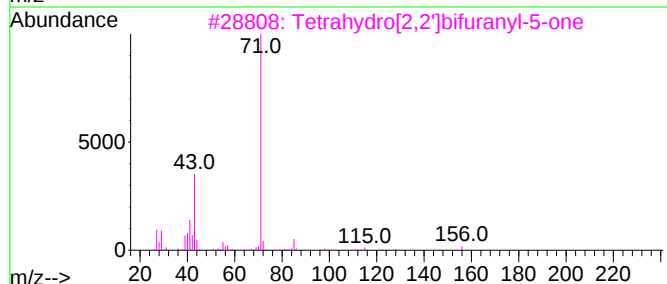
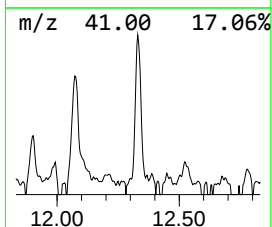
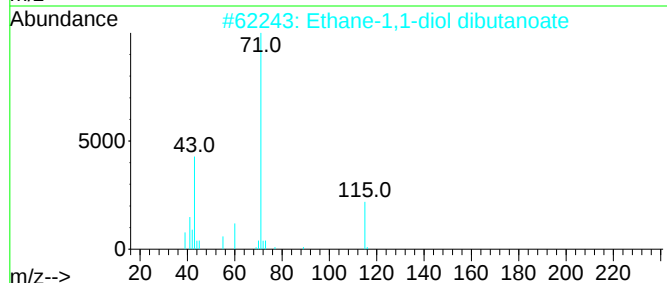
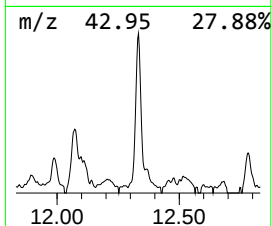
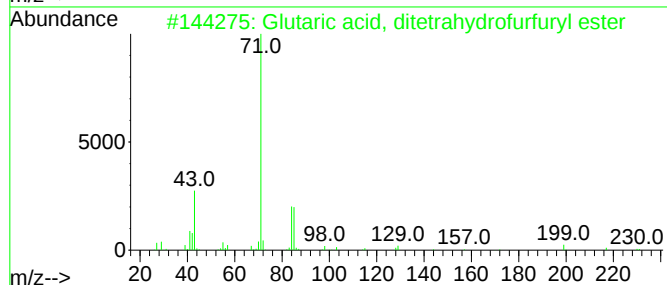
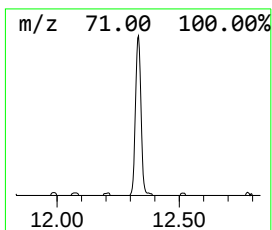
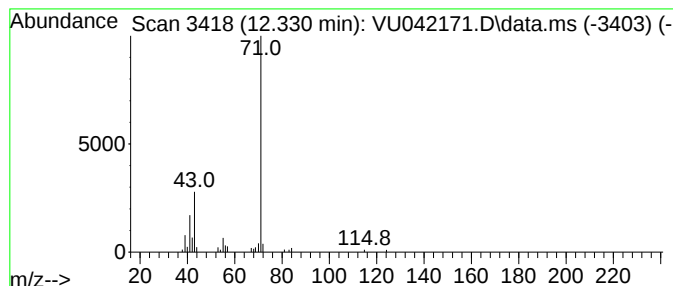
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Glutaric acid, ditetrahydro... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	0.56 ug/L	35346	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Glutaric acid, ditetrahydrofurfu...	300	C15H24O6	1000359-67-4	78
2			Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	64
3			Tetrahydro[2,2']bifuranyl-5-one	156	C8H12O3	019680-00-3	56
4			2,2'-Bifuran, octahydro-	142	C8H14O2	001592-33-2	56
5			Tetrahydrofuran, 2-propyl-	114	C7H14O	003208-22-8	56



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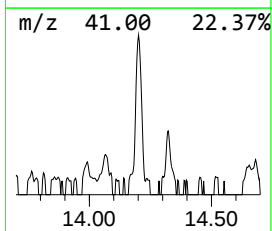
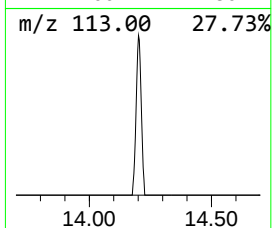
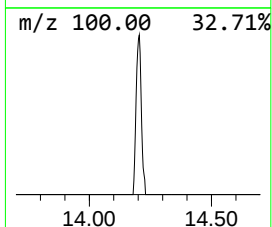
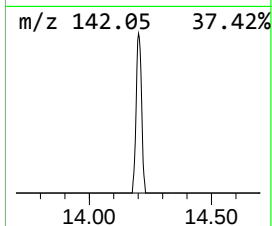
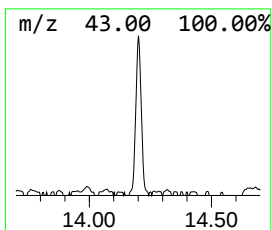
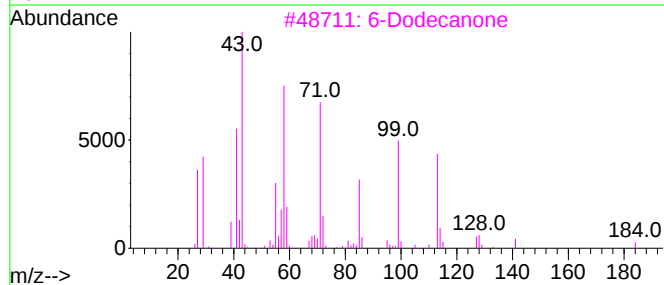
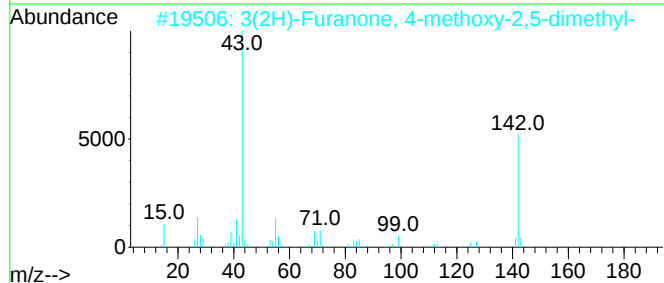
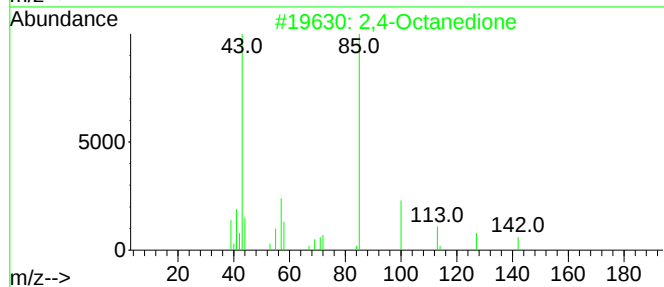
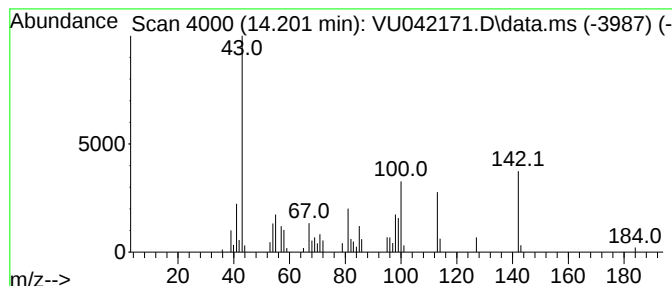
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Quant Title : TRACE VOA SOM01.0

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	0.60 ug/L	38276	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-Dodecanone	184	C12H24O	006064-27-3	35
4			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	32
5			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	25



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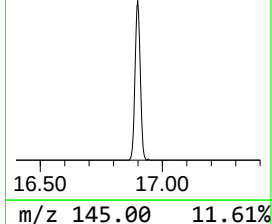
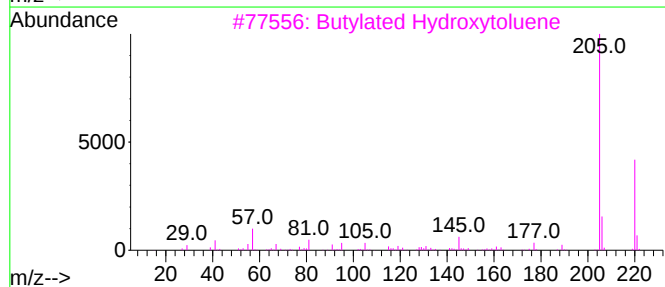
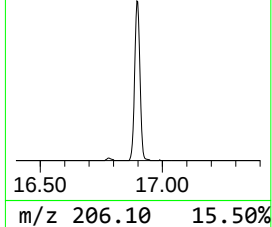
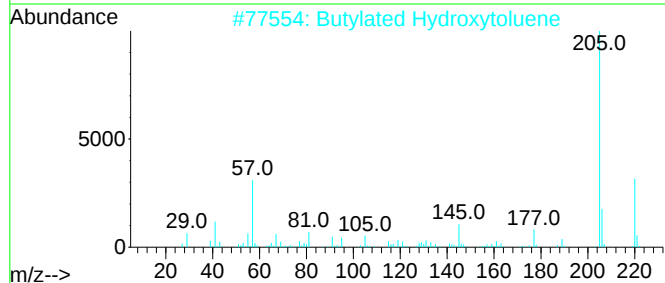
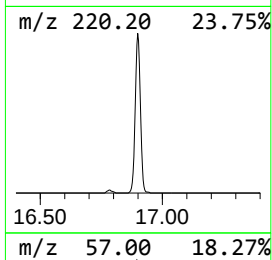
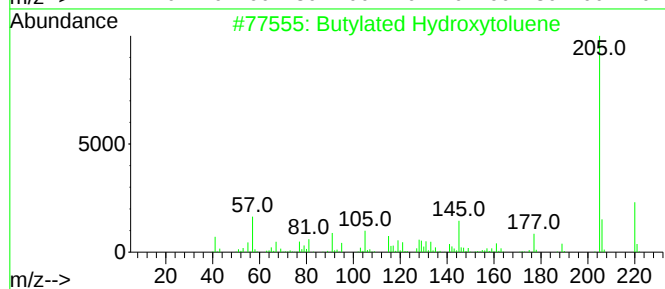
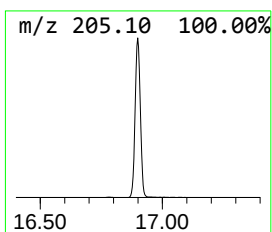
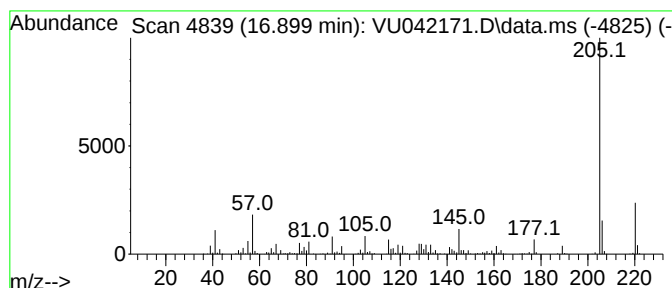
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	10.13 ug/L	641819	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	94
5			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93



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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	1.2	ug/L	56107	1	6.256	241478	5.0
Glutaric acid, ...	12.330	0.6	ug/L	35346	3	11.819	316906	5.0
unknown-01	14.201	0.6	ug/L	38276	3	11.819	316906	5.0
Butylated Hydro...	16.899	10.1	ug/L	641819	3	11.819	316906	5.0