

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
 Data File : VU042118.D
 Acq On : 20 Jan 2021 20:12
 Operator : SY/MD
 Sample : M1180-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F1E05

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: VU042118.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	7705	10523	2.17%	0.197%
2	1.488	40	46	52	rBV2	5554	6297	1.30%	0.118%
3	1.601	70	81	92	rBV2	57914	85383	17.59%	1.598%
4	1.919	171	180	190	rVB	42884	54450	11.22%	1.019%
5	2.337	300	310	320	rBV4	15542	29329	6.04%	0.549%
6	2.568	372	382	395	rVB	91127	147112	30.31%	2.754%
7	3.273	583	601	609	rBV2	8965	25460	5.25%	0.477%
8	4.459	956	970	989	rBV4	8486	23569	4.86%	0.441%
9	4.668	1017	1035	1089	rBV3	70214	249251	51.36%	4.666%
10	5.073	1142	1161	1179	rBV	79410	176803	36.43%	3.310%
11	5.732	1341	1366	1391	rBV2	160987	418607	86.26%	7.837%
12	6.176	1491	1504	1514	rBV2	2765	6747	1.39%	0.126%
13	6.256	1514	1529	1552	rVB	153771	285894	58.91%	5.352%
14	6.649	1639	1651	1655	rBV4	5338	8991	1.85%	0.168%
15	6.700	1655	1667	1687	rVB	103437	205408	42.33%	3.845%
16	7.176	1792	1815	1842	rBV	102570	218154	44.95%	4.084%
17	7.575	1925	1939	1956	rBV	59581	106908	22.03%	2.001%
18	7.838	2002	2021	2031	rBV4	15141	39063	8.05%	0.731%
19	7.906	2031	2042	2057	rVV	200383	348974	71.91%	6.533%
20	7.980	2059	2065	2074	rVV6	3241	6508	1.34%	0.122%
21	8.041	2074	2084	2097	rVB2	8959	16603	3.42%	0.311%
22	8.189	2118	2130	2143	rBV2	38450	67483	13.91%	1.263%
23	8.497	2212	2226	2238	rBV	15847	29166	6.01%	0.546%
24	8.558	2238	2245	2253	rVB4	3791	5655	1.17%	0.106%
25	8.645	2259	2272	2292	rBV	251674	485302	100.00%	9.085%
26	8.796	2313	2319	2335	rVB4	5036	9260	1.91%	0.173%
27	9.427	2503	2515	2533	rBV	208958	361889	74.57%	6.775%
28	9.648	2576	2584	2595	rVB2	30544	48069	9.90%	0.900%
29	9.771	2611	2622	2641	rBV3	7445	17336	3.57%	0.325%
30	9.928	2655	2671	2682	rBV4	6804	13131	2.71%	0.246%
31	10.041	2700	2706	2717	rVB5	3687	6199	1.28%	0.116%
32	10.353	2795	2803	2812	rBV6	3899	6931	1.43%	0.130%
33	10.652	2886	2896	2901	rBV5	5511	9183	1.89%	0.172%
34	10.693	2901	2909	2920	rVV2	13181	21611	4.45%	0.405%
35	10.764	2920	2931	2943	rVV	79080	125540	25.87%	2.350%
36	10.899	2967	2973	2981	rVB4	4741	7311	1.51%	0.137%

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37	10.973	2981	2996	3010	rBV	15421	28181	5.81%	0.528%
38	11.063	3010	3024	3032	rVV6	4825	9041	1.86%	0.169%
39	11.478	3147	3153	3163	rVB4	3535	5284	1.09%	0.099%
40	11.697	3212	3221	3231	rVB7	4886	8483	1.75%	0.159%
41	11.819	3247	3259	3276	rBV	224383	359139	74.00%	6.723%
42	11.986	3305	3311	3324	rVB3	7481	12708	2.62%	0.238%
43	12.073	3327	3338	3360	rBV	37380	83576	17.22%	1.565%
44	12.201	3366	3378	3392	rVB	203125	325642	67.10%	6.096%
45	12.333	3406	3419	3432	rBV2	10197	17726	3.65%	0.332%
46	12.526	3469	3479	3496	rVB6	6804	15506	3.20%	0.290%
47	12.896	3585	3594	3603	rVB8	4680	7582	1.56%	0.142%
48	12.957	3603	3613	3624	rBV2	10361	15171	3.13%	0.284%
49	13.619	3810	3819	3825	rVB7	3427	5510	1.14%	0.103%
50	14.201	3988	4000	4012	rBV	75811	113211	23.33%	2.119%
51	14.327	4029	4039	4051	rBV2	16144	22525	4.64%	0.422%
52	15.012	4238	4252	4260	rBV4	8635	15642	3.22%	0.293%
53	15.462	4384	4392	4401	rBV2	5202	7355	1.52%	0.138%
54	15.555	4414	4421	4427	rBV5	3978	5211	1.07%	0.098%
55	15.597	4427	4434	4442	rVB7	4496	7148	1.47%	0.134%
56	15.706	4458	4468	4481	rVB3	13780	23679	4.88%	0.443%
57	16.143	4594	4604	4613	rBV2	21679	34556	7.12%	0.647%
58	16.285	4639	4648	4653	rBV6	3342	5086	1.05%	0.095%
59	16.780	4793	4802	4816	rBV3	33654	55527	11.44%	1.039%
60	16.899	4828	4839	4851	rBV	325030	474168	97.71%	8.877%

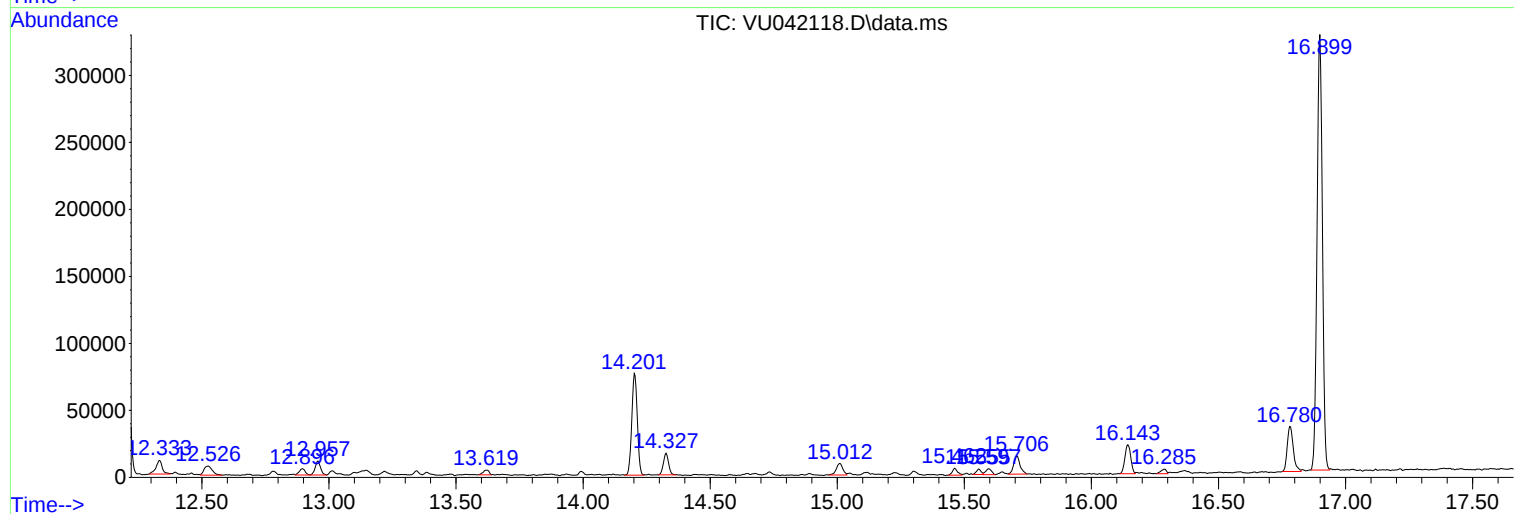
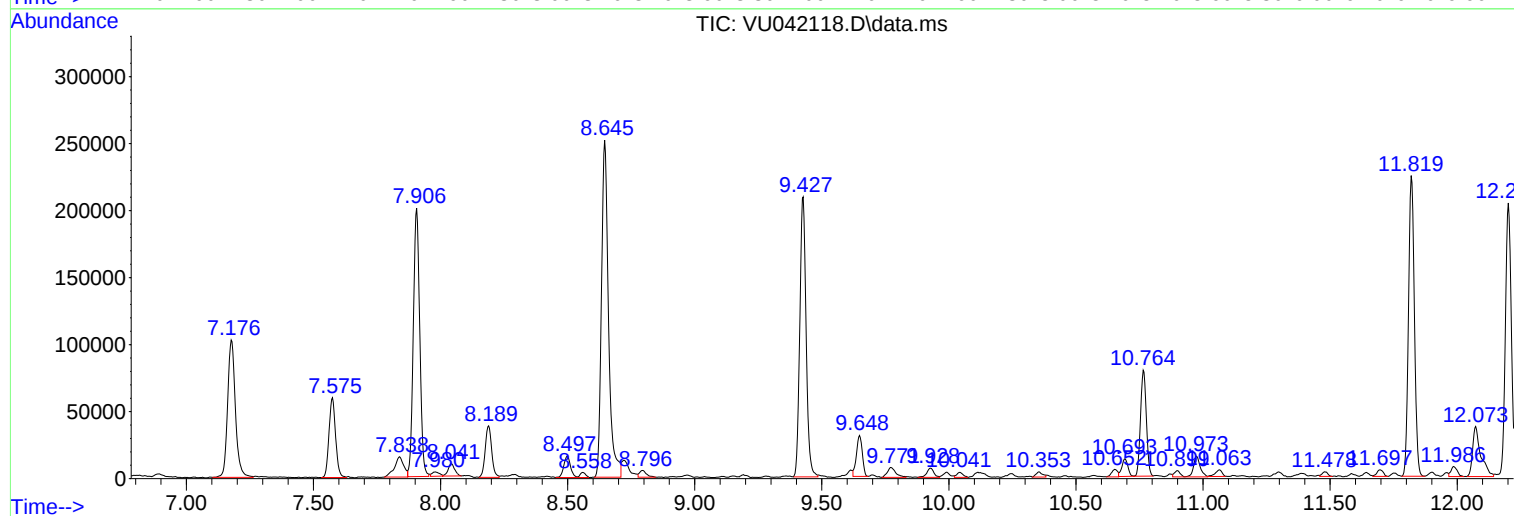
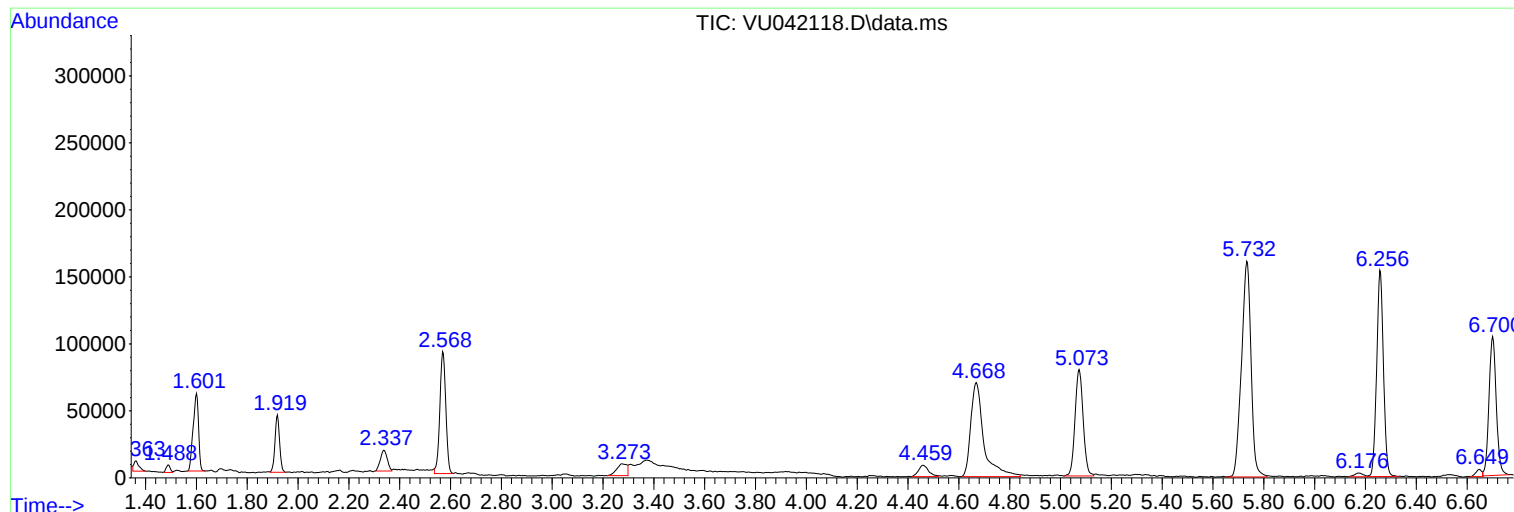
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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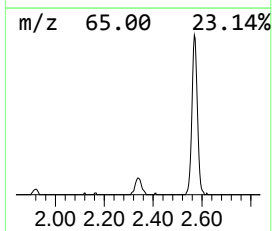
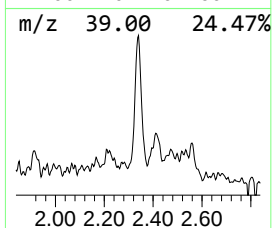
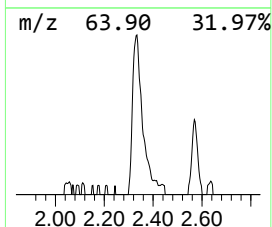
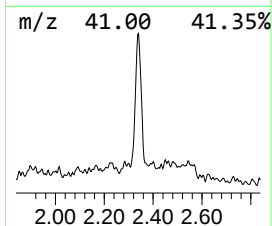
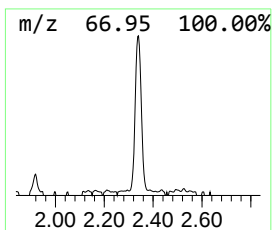
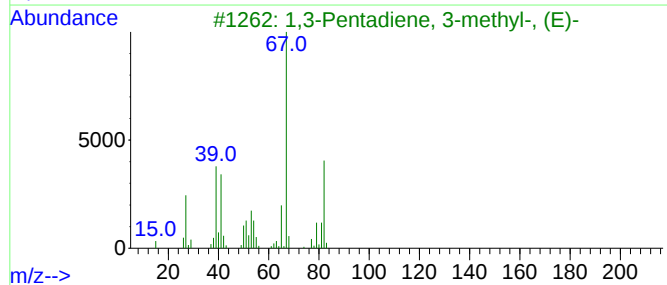
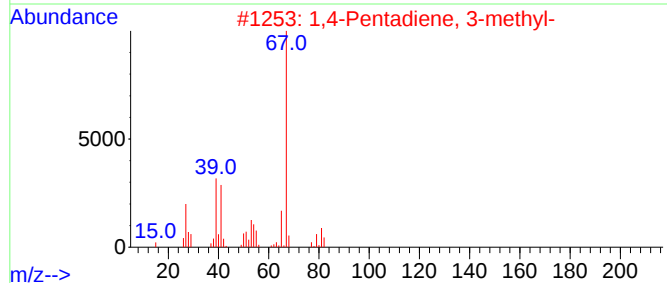
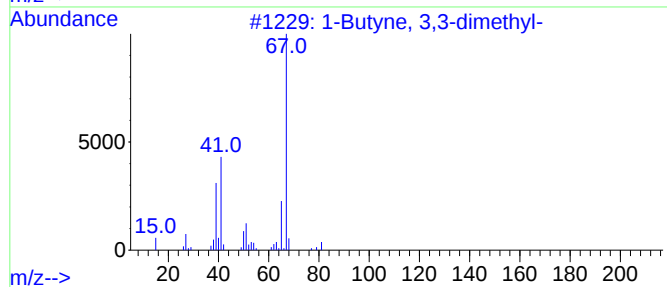
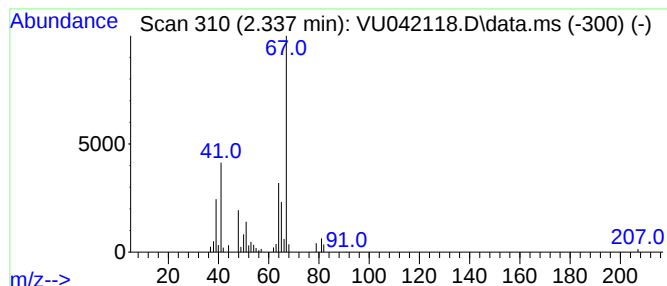
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 1-Butyne, 3,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.337	0.51 ug/L	29329	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	50
2			1,4-Pentadiene, 3-methyl-	82	C6H10	001115-08-8	47
3			1,3-Pentadiene, 3-methyl-, (E)-	82	C6H10	002787-43-1	42
4			1,3-Butadiene, 2-(bromomethyl)-	146	C5H7Br	023691-13-6	40
5			1,4-Pentadiene, 2-methyl-	82	C6H10	000763-30-4	38



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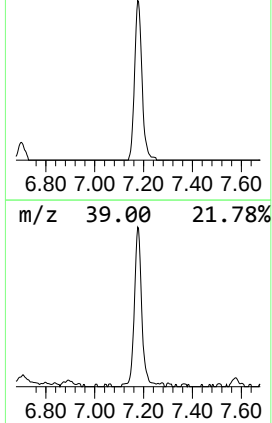
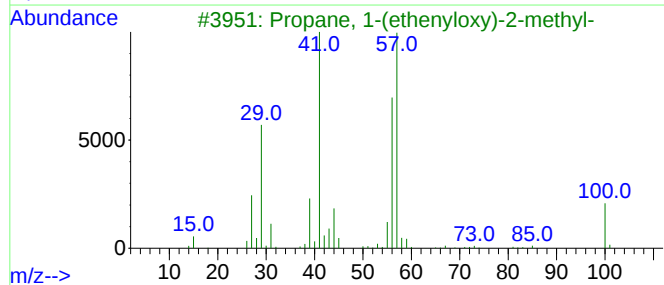
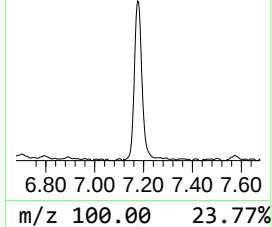
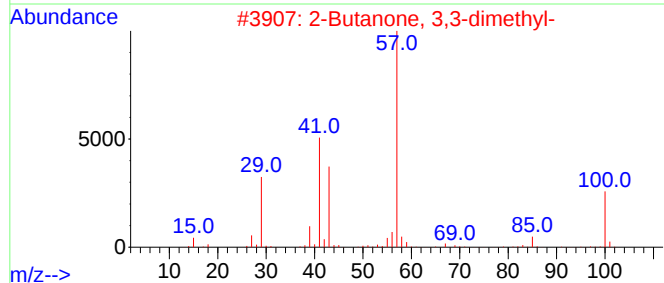
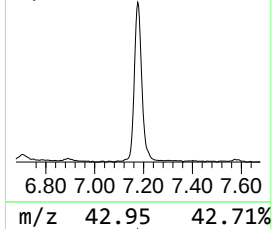
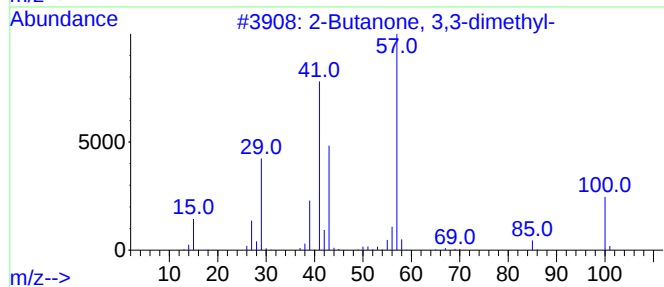
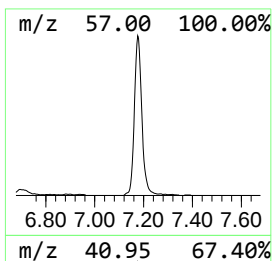
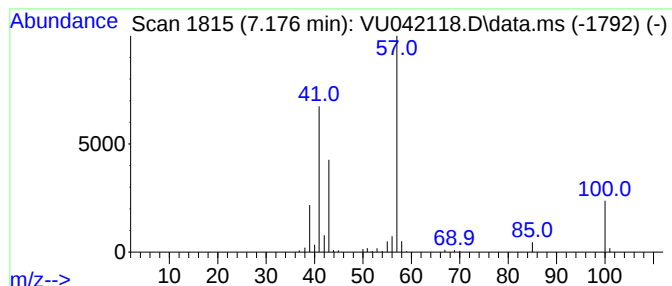
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.176	3.82 ug/L	218154	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	90
3	Propane, 1-(ethenyloxy)-2-methyl-			100	C6H12O	000109-53-5	59
4	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	53
5	3-Hexanone			100	C6H12O	000589-38-8	50



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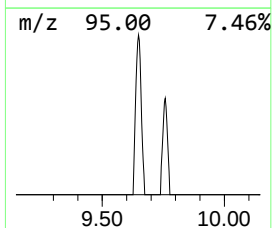
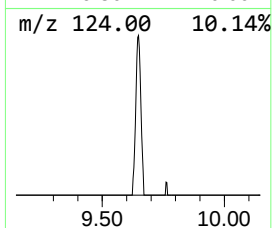
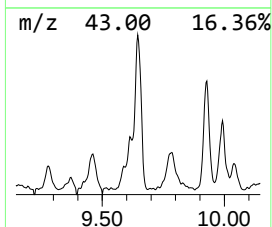
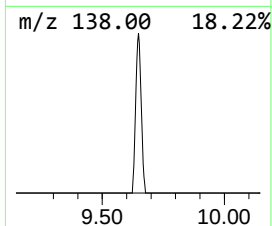
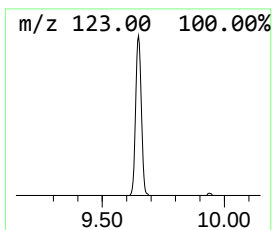
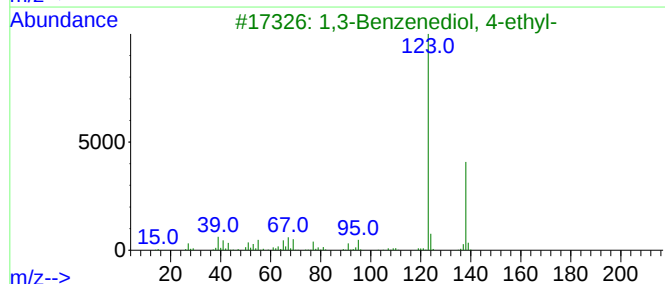
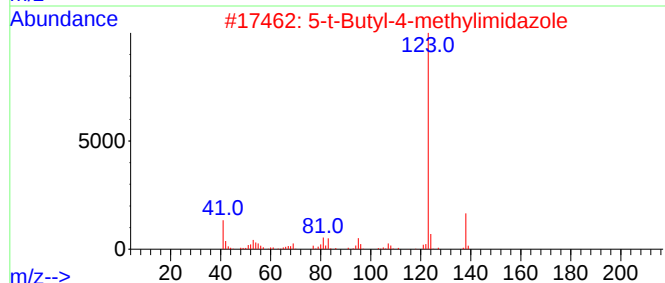
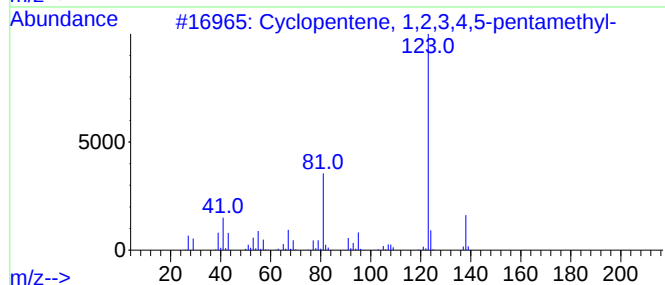
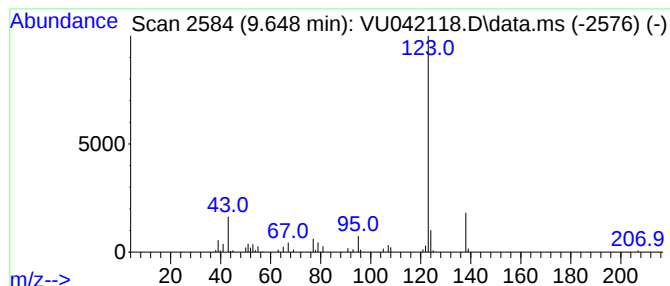
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Cyclopentene, 1,2,3,4,5-pen... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.648	0.66 ug/L	48069	Chlorobenzene-d5	9.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentene, 1,2,3,4,5-pentamet...	138	C10H18	1000154-28-6	91
2			5-t-Butyl-4-methylimidazole	138	C8H14N2	146979-50-2	90
3			1,3-Benzenediol, 4-ethyl-	138	C8H10O2	002896-60-8	86
4			Cyclopentene, 1,2,3,3,4-pentamet...	138	C10H18	197390-29-7	83
5			Benzene, 1,4-dimethoxy-	138	C8H10O2	000150-78-7	78



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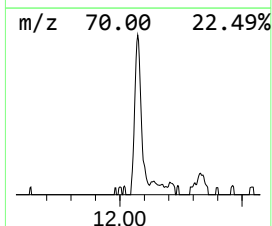
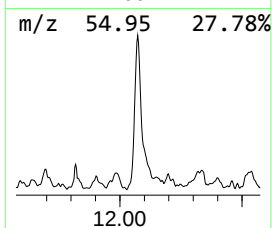
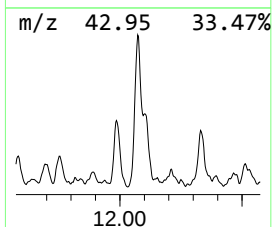
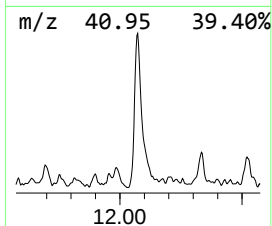
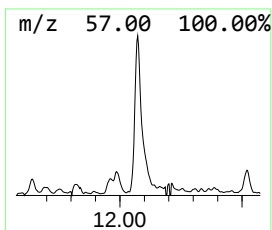
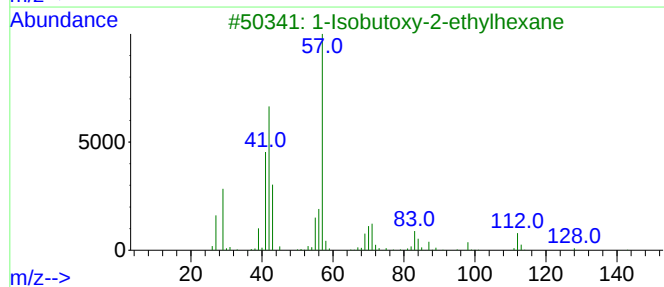
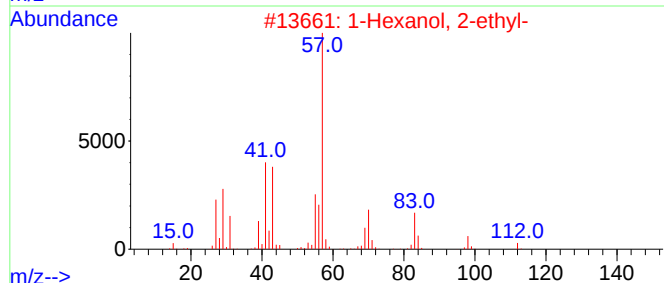
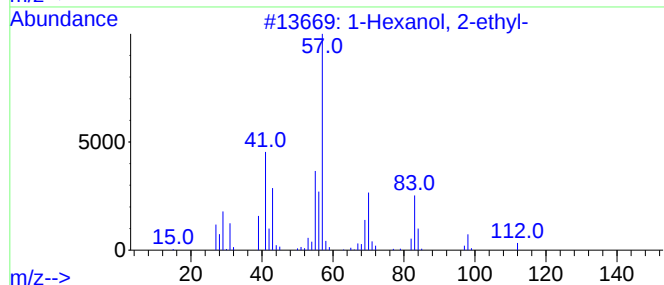
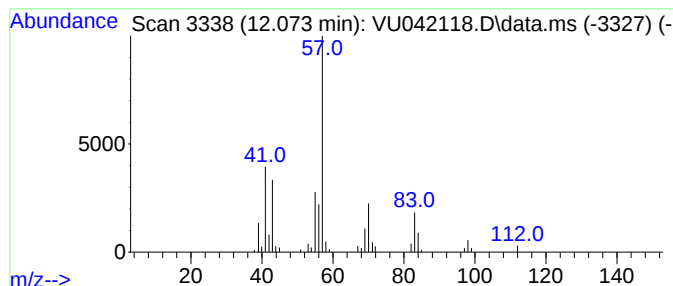
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.073	1.16 ug/L	83576	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E05

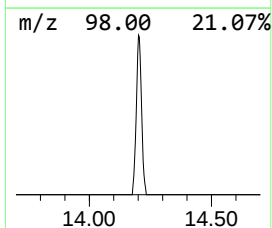
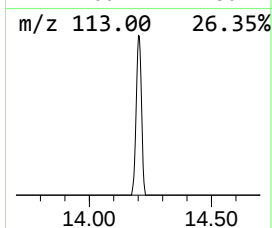
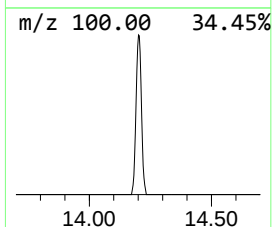
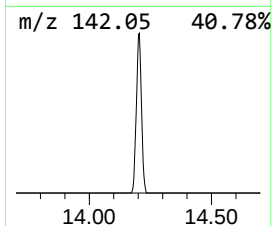
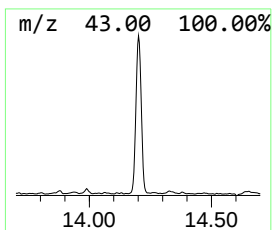
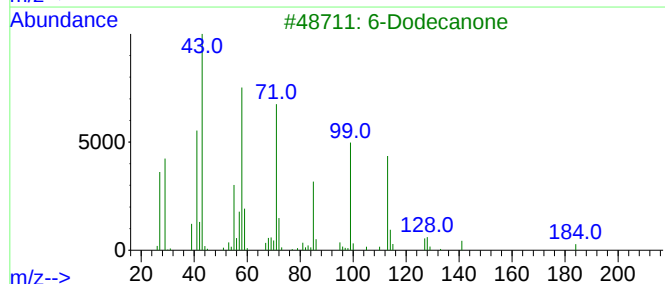
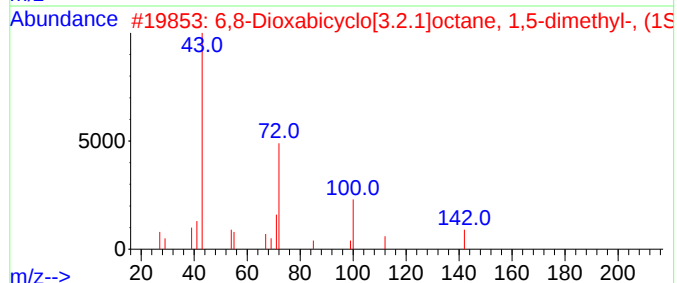
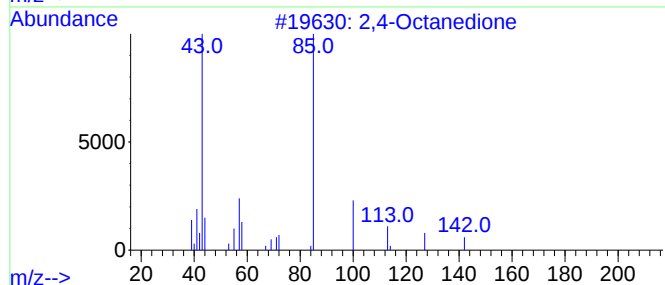
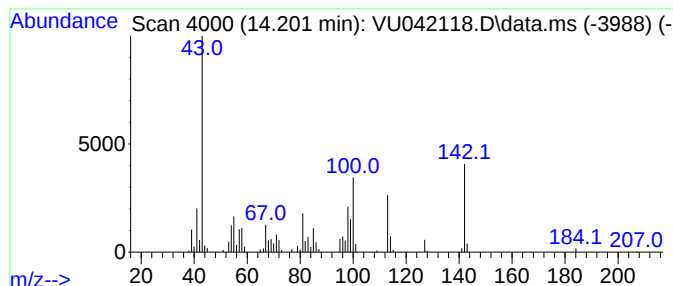
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	1.58 ug/L	113211	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	47
2			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	32
3			6-Dodecanone	184	C12H24O	006064-27-3	14
4			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	12
5			6-Dodecanone	184	C12H24O	006064-27-3	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042118.D
Acq On : 20 Jan 2021 20:12
Operator : SY/MD
Sample : M1180-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E05

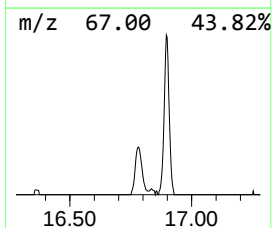
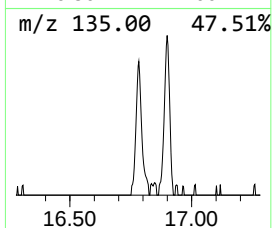
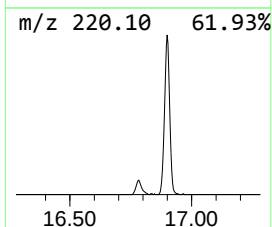
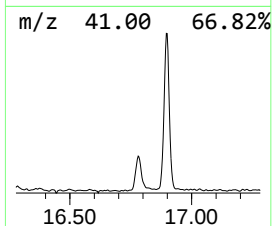
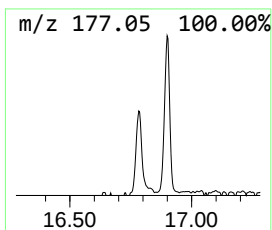
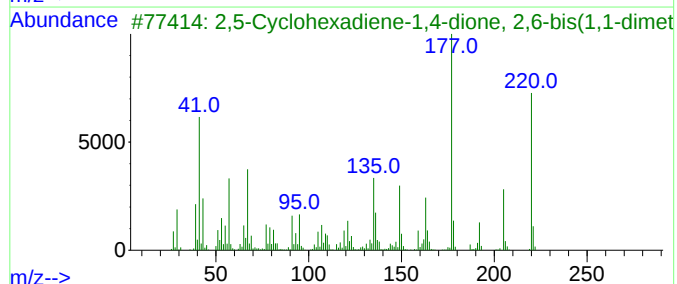
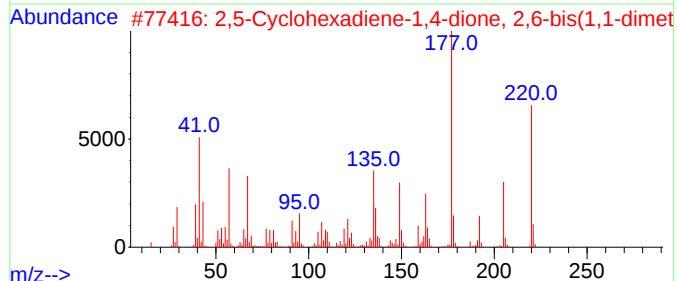
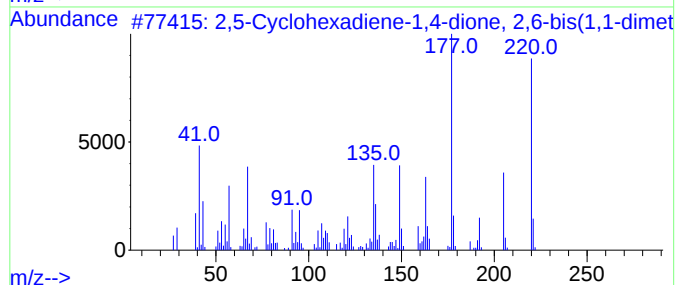
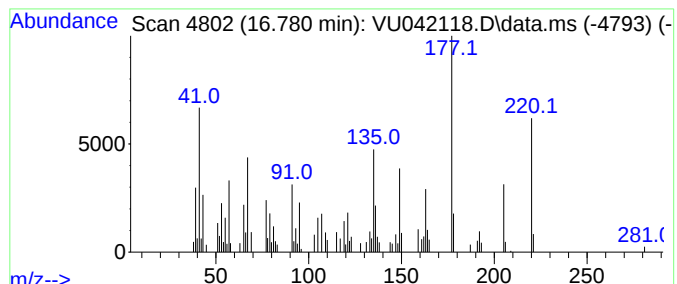
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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.
16.780	0.77 ug/L	55527	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
4			Octamethyl-1,4-cyclohexadiene	192	C14H24	172684-93-4	38
5			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042118.D
Acq On : 20 Jan 2021 20:12
Operator : SY/MD
Sample : M1180-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E05

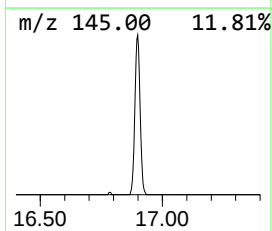
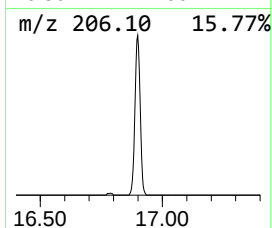
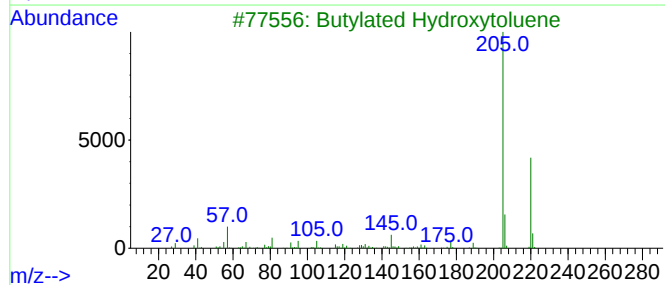
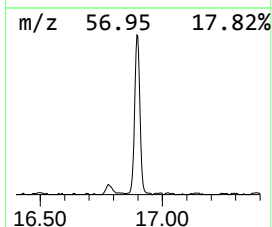
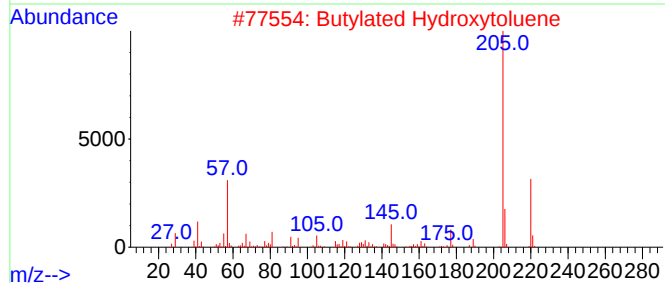
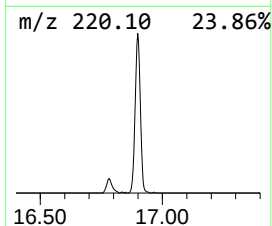
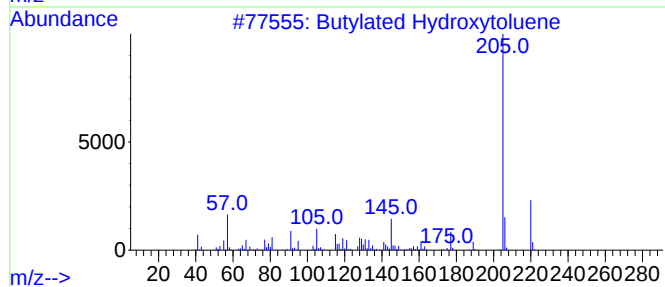
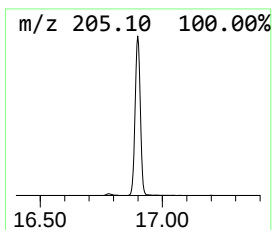
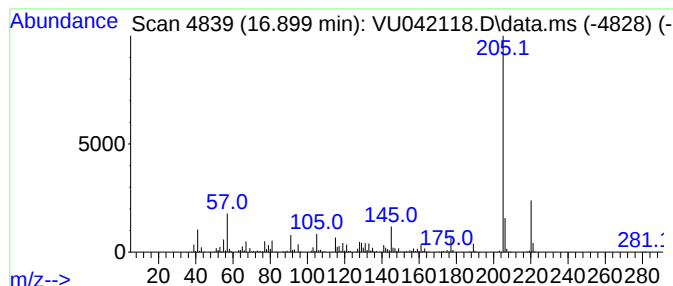
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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	6.60 ug/L	474168	1,4-Dichlorobenzene-d4	11.822

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012021\
Data File : VU042118.D
Acq On : 20 Jan 2021 20:12
Operator : SY/MD
Sample : M1180-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F1E05

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
1-Butyne, 3,3-d...	2.337	0.5	ug/L	29329	1	6.256	285894	5.0
2-Butanone, 3,3...	7.176	3.8	ug/L	218154	1	6.256	285894	5.0
Cyclopentene, 1...	9.648	0.7	ug/L	48069	2	9.427	361889	5.0
1-Hexanol, 2-et...	12.073	1.2	ug/L	83576	3	11.822	359139	5.0
unknown-01	14.201	1.6	ug/L	113211	3	11.822	359139	5.0
2,5-Cyclohexadi...	16.780	0.8	ug/L	55527	3	11.822	359139	5.0
Butylated Hydro...	16.899	6.6	ug/L	474168	3	11.822	359139	5.0