

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091420\
 Data File : VU040118.D
 Acq On : 14 Sep 2020 14:04
 Operator : SY/MD
 Sample : L3961-18
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4Y43

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

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	20	rBV3	6725	7386	1.60%	0.185%
2	1.604	70	82	97	rVB2	53087	76029	16.51%	1.905%
3	1.765	109	132	133	rBV2	42858	117163	25.44%	2.935%
4	1.922	176	181	196	rVB	47190	64725	14.06%	1.621%
5	2.581	374	386	398	rBV	86315	140239	30.45%	3.513%
6	2.688	401	419	434	rBV2	15669	65704	14.27%	1.646%
7	3.379	626	634	635	rBV5	5991	6762	1.47%	0.169%
8	3.800	758	765	780	rVB8	3238	5778	1.25%	0.145%
9	4.520	973	989	1005	rBV4	13476	35692	7.75%	0.894%
10	4.668	1017	1035	1075	rBV	45061	195949	42.55%	4.909%
11	4.832	1075	1086	1105	rVB3	16206	43131	9.37%	1.080%
12	5.083	1150	1164	1181	rBV2	73727	161998	35.18%	4.058%
13	5.601	1310	1325	1337	rBV5	7682	15615	3.39%	0.391%
14	5.742	1348	1369	1384	rBV2	143035	366161	79.51%	9.172%
15	6.263	1516	1531	1550	rBV	168272	311887	67.73%	7.813%
16	6.507	1597	1607	1621	rBV2	10907	20380	4.43%	0.511%
17	6.703	1655	1668	1684	rBV2	90118	173348	37.64%	4.342%
18	7.575	1927	1939	1952	rBV2	44813	77902	16.92%	1.951%
19	7.906	2027	2042	2057	rBV	160894	280005	60.80%	7.014%
20	8.186	2118	2129	2140	rBV	26503	45803	9.95%	1.147%
21	8.642	2257	2271	2296	rBV	244313	460502	100.00%	11.536%
22	8.951	2353	2367	2372	rBV5	4315	9168	1.99%	0.230%
23	9.420	2500	2513	2533	rBV	245669	406292	88.23%	10.178%
24	10.234	2753	2766	2777	rBV3	5067	8080	1.75%	0.202%
25	10.755	2914	2928	2944	rVB	71133	120418	26.15%	3.016%
26	11.472	3141	3151	3164	rBV3	9066	14627	3.18%	0.366%
27	11.806	3244	3255	3270	rBV	238577	381579	82.86%	9.559%
28	12.054	3321	3332	3345	rBV2	49898	85247	18.51%	2.135%
29	12.189	3362	3374	3386	rVB	175829	281797	61.19%	7.059%
30	12.768	3543	3554	3562	rBV5	4642	6934	1.51%	0.174%
31	13.198	3682	3688	3699	rVB3	4319	5725	1.24%	0.143%

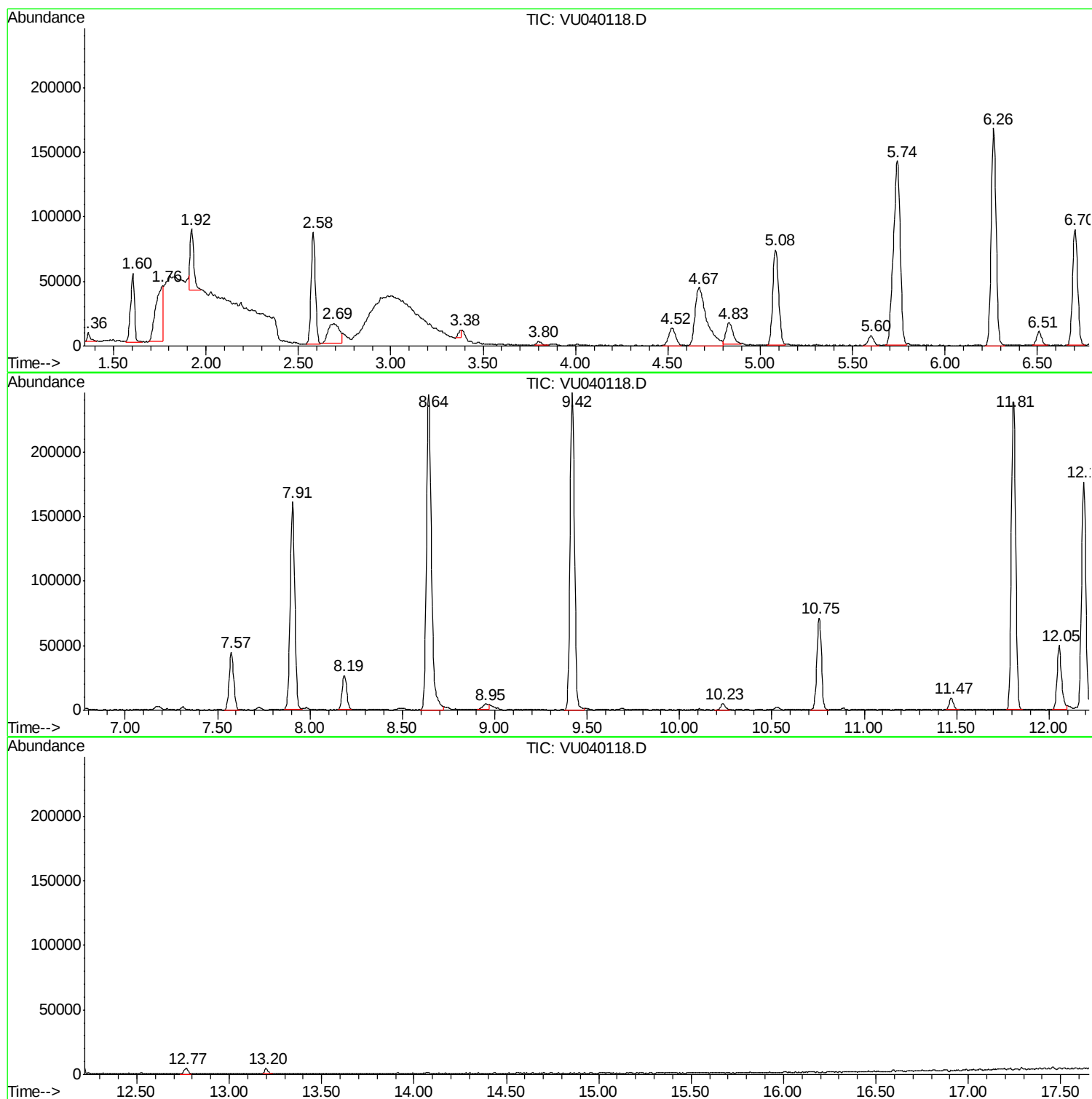
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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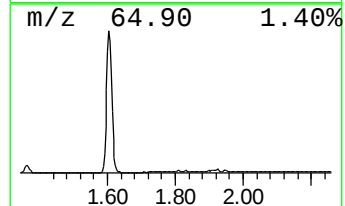
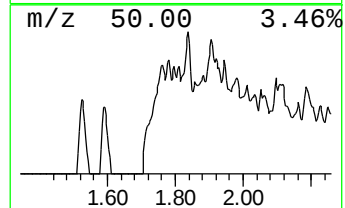
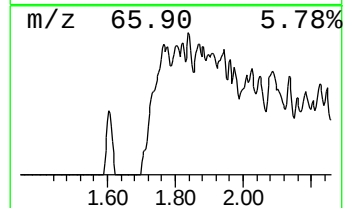
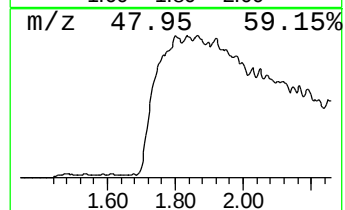
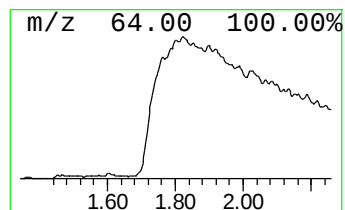
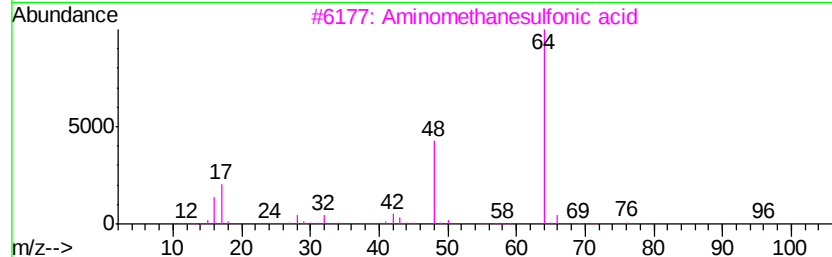
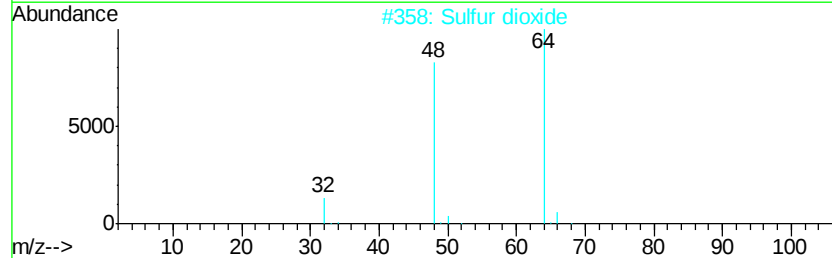
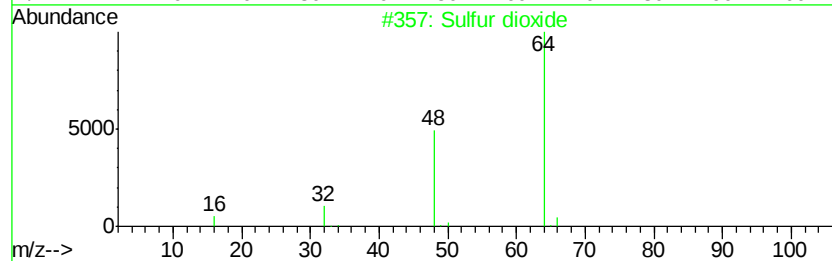
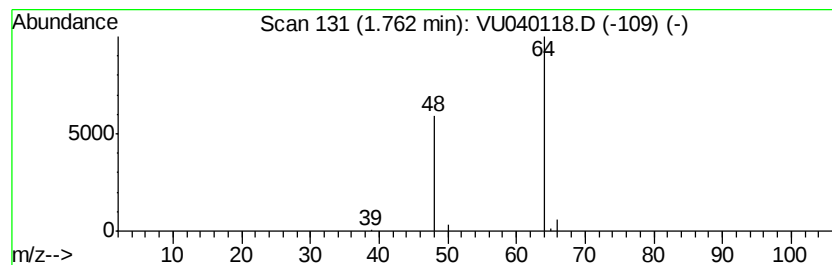
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.76	1.88 ug/L	117163	1,4-Difluorobenzene	6.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 02S	007446-09-5	90
2	Sulfur dioxide	64 02S	007446-09-5	74
3	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	64
4	L-Alanine, 3-sulfo-	169 C3H7N05S	000498-40-8	9
5	Aminomethanesulfonic acid	111 CH5N03S	013881-91-9	9



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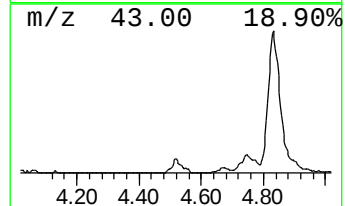
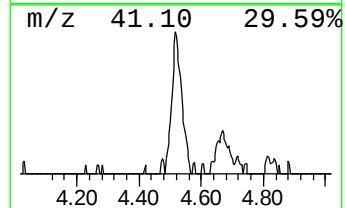
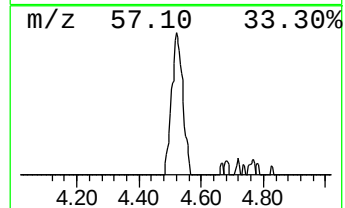
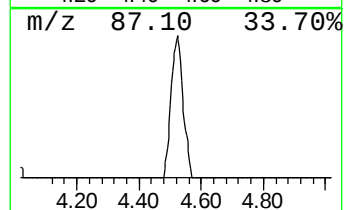
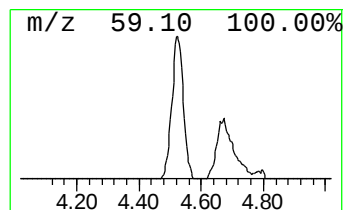
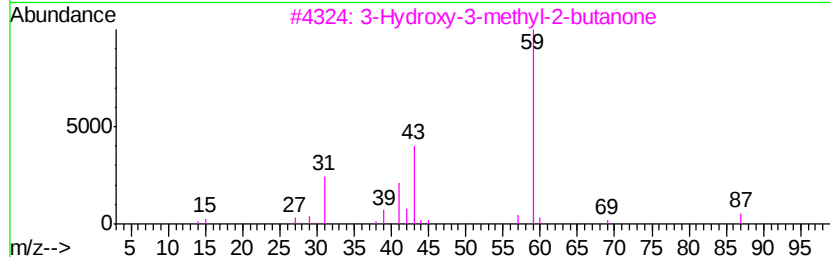
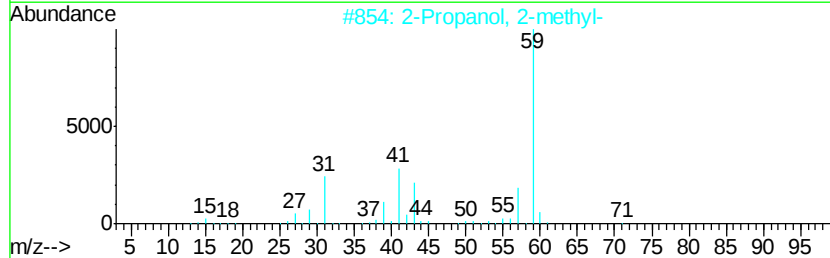
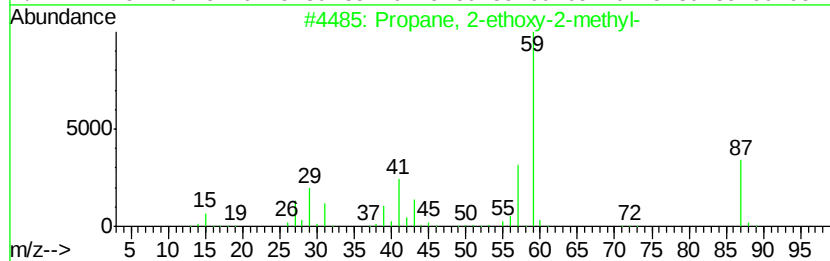
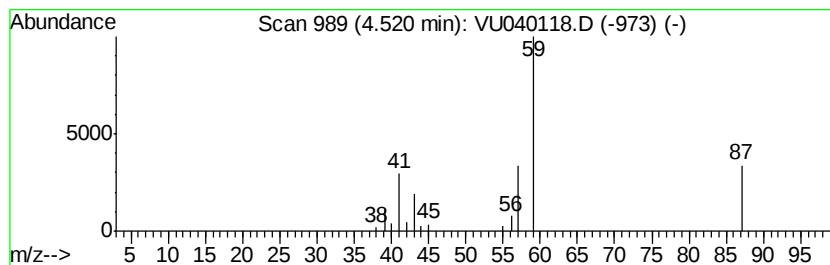
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Propane, 2-ethoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	0.57 ug/L	35692	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	74
2		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



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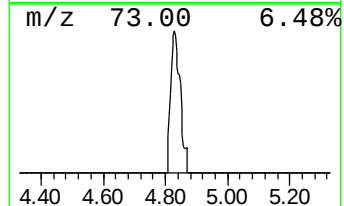
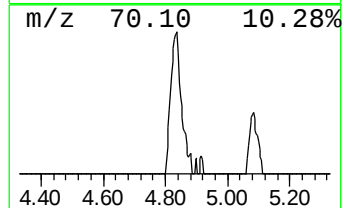
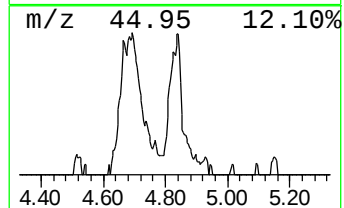
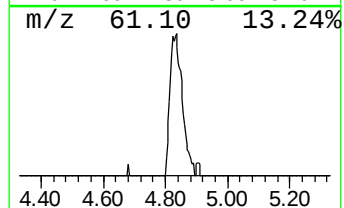
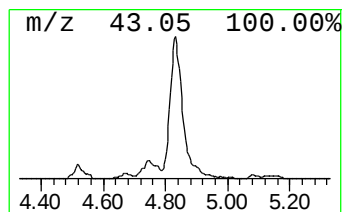
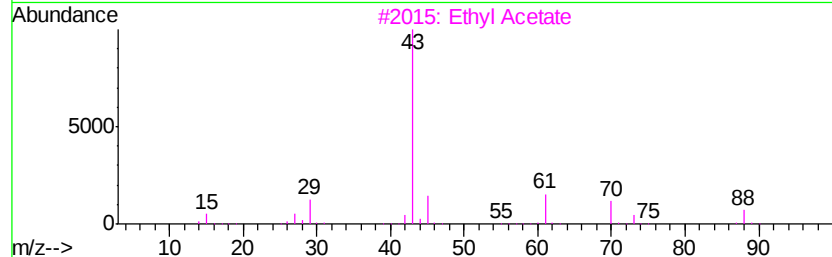
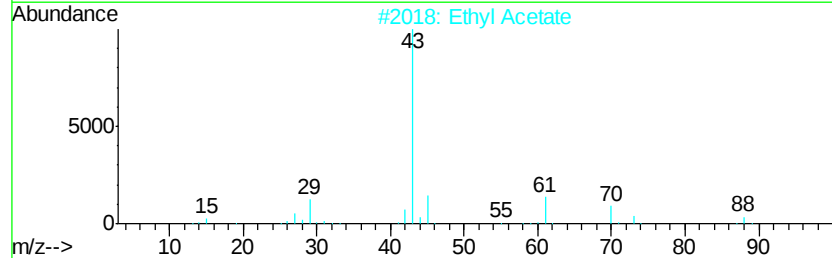
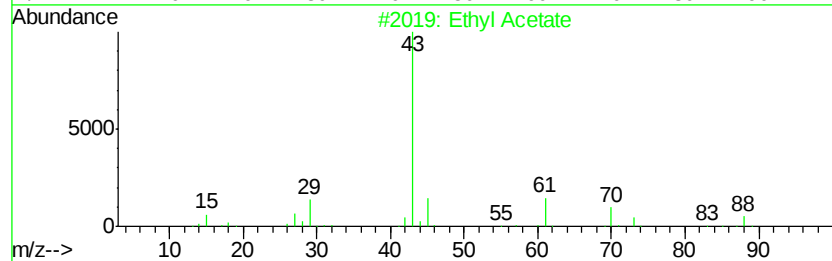
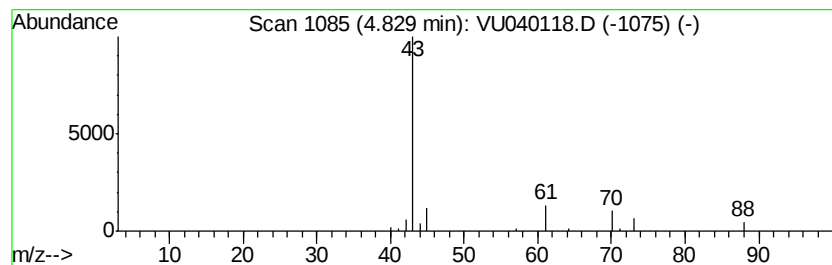
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.69 ug/L	43131	1,4-Difluorobenzene	6.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	83
4			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	59
5			Ethyl Acetate	88	C4H8O2	000141-78-6	45



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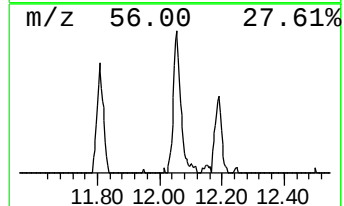
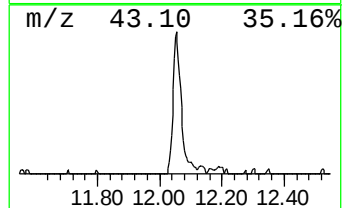
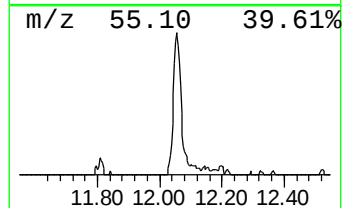
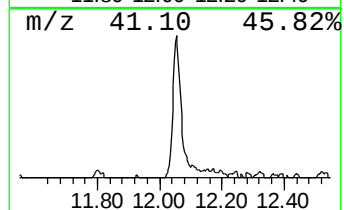
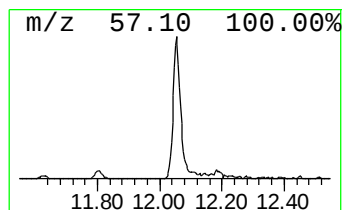
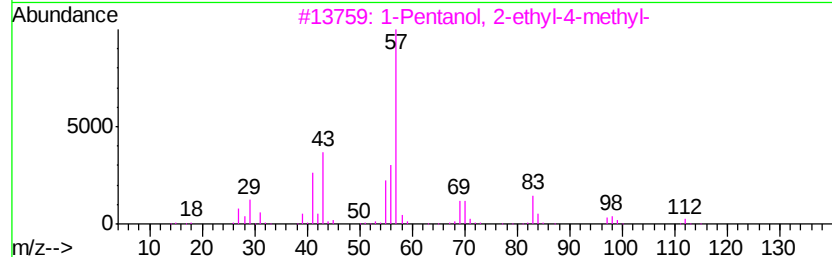
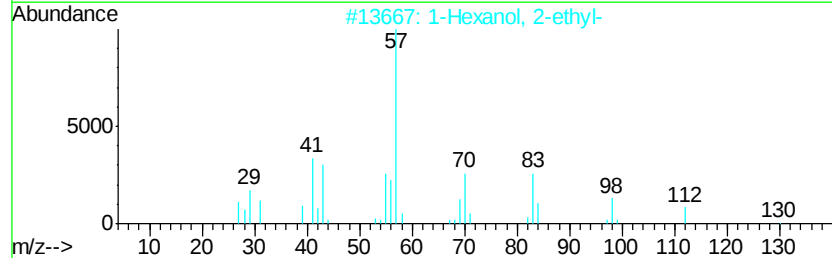
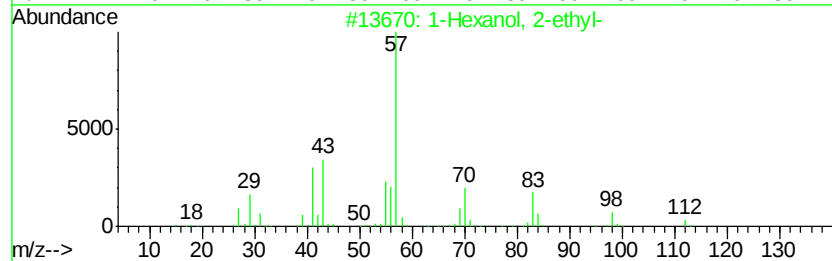
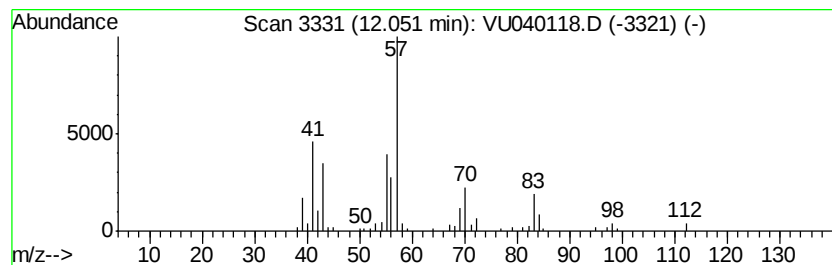
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Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.05	1.12 ug/L	85247	1,4-Dichlorobenzene-d4	11.81	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.76	1.9	ug/L	117163	1	6.26	311887	5.0
Propane, 2-ethoxy...	4.52	0.6	ug/L	35692	1	6.26	311887	5.0
Ethyl Acetate	4.83	0.7	ug/L	43131	1	6.26	311887	5.0
1-Hexanol, 2-ethyl-	12.05	1.1	ug/L	85247	3	11.81	381579	5.0