

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100220\
 Data File : VU040464.D
 Acq On : 02 Oct 2020 16:32
 Operator : SY/MD
 Sample : L4185-09
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AT2

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\SOMUTR092920WMA.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	1.527	52	58	61	rBV	6950	7881	1.65%	0.178%
2	1.607	75	83	92	rVB	48251	54959	11.53%	1.242%
3	1.922	174	181	194	rVB	38679	49751	10.43%	1.125%
4	2.581	374	386	399	rBV	77624	129112	27.08%	2.919%
5	2.658	399	410	431	rVV	13669	34838	7.31%	0.788%
6	2.842	445	467	469	rBV3	3991	10437	2.19%	0.236%
7	3.096	539	546	556	rVB6	3353	6128	1.29%	0.139%
8	3.379	619	634	646	rVB3	5248	11326	2.38%	0.256%
9	3.597	681	702	717	rBV2	23581	55885	11.72%	1.263%
10	3.716	726	739	754	rVB3	13304	29691	6.23%	0.671%
11	3.977	809	820	833	rBV2	2459	5827	1.22%	0.132%
12	4.552	987	999	1007	rBV6	2959	6127	1.28%	0.139%
13	4.652	1014	1030	1069	rBV	67839	210982	44.25%	4.770%
14	4.825	1069	1084	1111	rVV	104408	249350	52.29%	5.637%
15	5.083	1148	1164	1189	rBV3	88908	212107	44.48%	4.795%
16	5.739	1347	1368	1396	rBV3	145265	386872	81.13%	8.746%
17	6.263	1517	1531	1551	rBV	173939	326892	68.56%	7.390%
18	6.703	1655	1668	1684	rBV2	94313	179653	37.68%	4.061%
19	7.173	1797	1814	1832	rVB8	3127	8060	1.69%	0.182%
20	7.575	1926	1939	1952	rBV2	48457	83880	17.59%	1.896%
21	7.723	1971	1985	2000	rVB2	27301	50502	10.59%	1.142%
22	7.906	2026	2042	2055	rBV	172599	295780	62.03%	6.687%
23	7.976	2055	2064	2082	rVB	31652	53846	11.29%	1.217%
24	8.185	2118	2129	2144	rBV	31233	53396	11.20%	1.207%
25	8.639	2258	2270	2296	rBV	259114	476827	100.00%	10.779%
26	8.790	2307	2317	2327	rBV2	31184	51159	10.73%	1.157%
27	9.420	2500	2513	2538	rBV	253397	422010	88.50%	9.540%
28	9.684	2586	2595	2608	rVB4	3439	5568	1.17%	0.126%
29	10.234	2752	2766	2779	rBV5	3891	7820	1.64%	0.177%
30	10.340	2789	2799	2809	rVB4	3740	5920	1.24%	0.134%
31	10.755	2917	2928	2943	rVB	74409	119187	25.00%	2.694%
32	10.890	2961	2970	2984	rVB4	3209	5120	1.07%	0.116%
33	11.468	3141	3150	3160	rBV4	4385	7255	1.52%	0.164%
34	11.684	3208	3217	3224	rVB7	4088	5513	1.16%	0.125%

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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\SOMUTR092920WMA.M
Title : TRACE VOA SOM01.0

35	11.809	3243	3256	3271	rVB	248092	401803	84.27%	9.083%
36	12.060	3323	3334	3352	rBV3	13445	29513	6.19%	0.667%
37	12.189	3360	3374	3387	rVB	176115	284949	59.76%	6.442%
38	12.880	3580	3589	3598	rBV4	11183	15838	3.32%	0.358%
39	13.201	3678	3689	3704	rBV	47877	71765	15.05%	1.622%

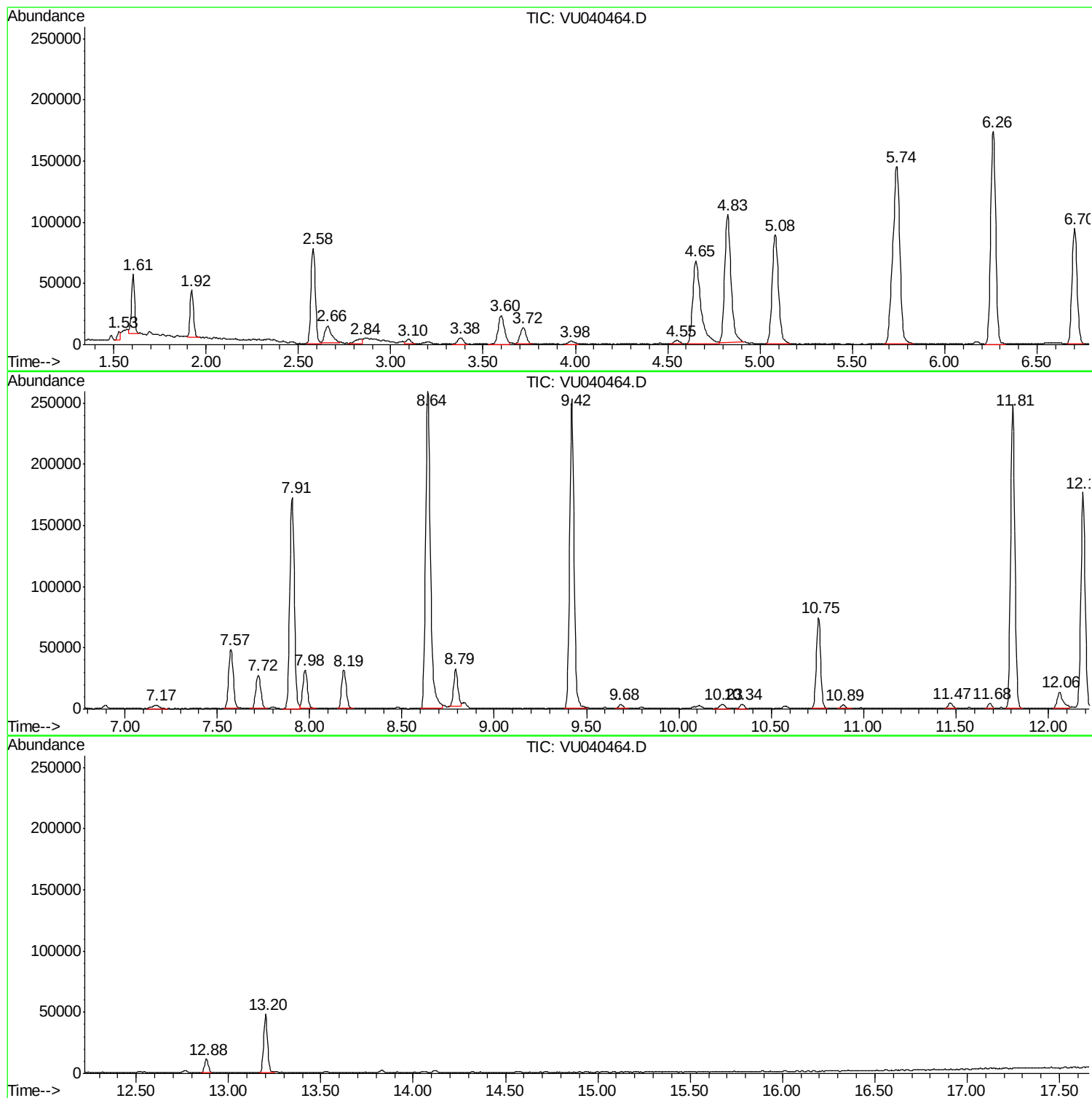
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Quant Title : TRACE VOA SOM01.0

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



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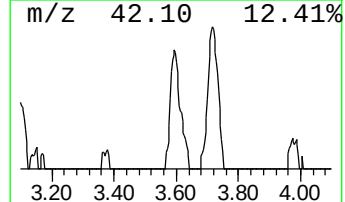
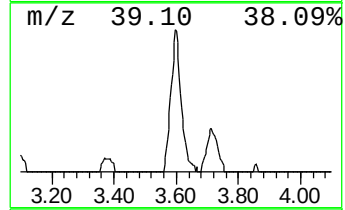
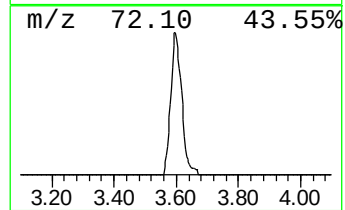
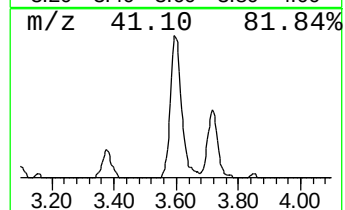
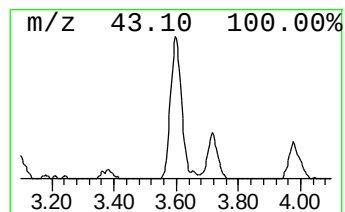
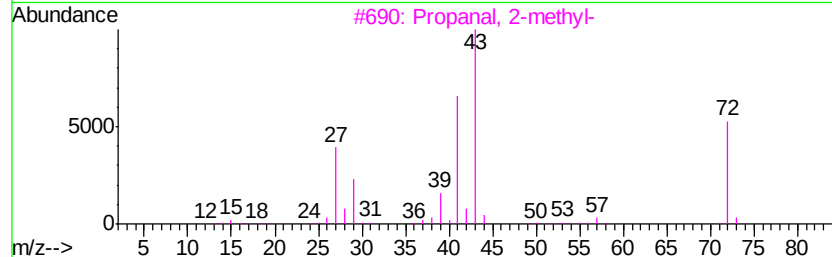
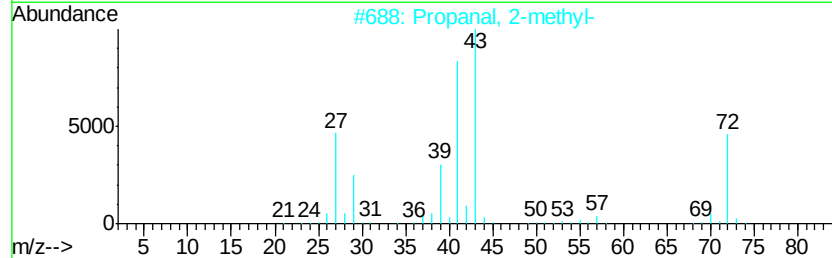
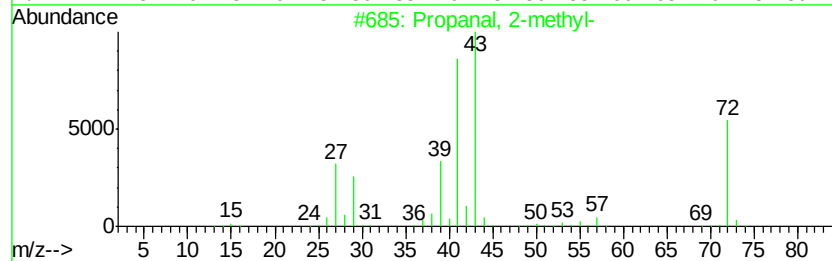
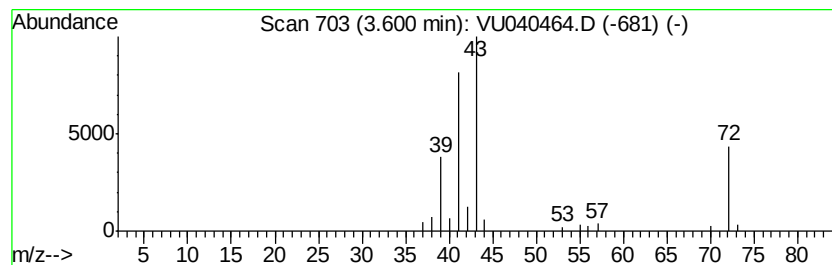
Instrument :
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ClientSampleId :
C0AT2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Propanal, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.60	0.85 ug/L	55885	1,4-Difluorobenzene	6.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	64
4	Butanal	72	C4H8O	000123-72-8	53
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	50



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Instrument :
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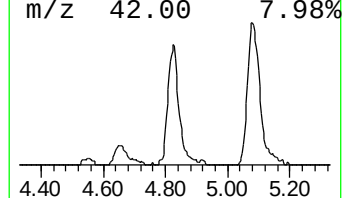
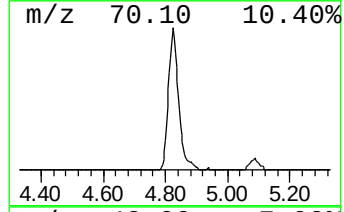
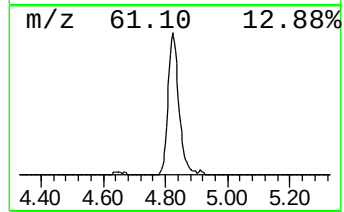
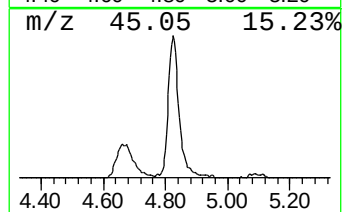
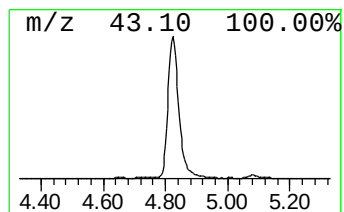
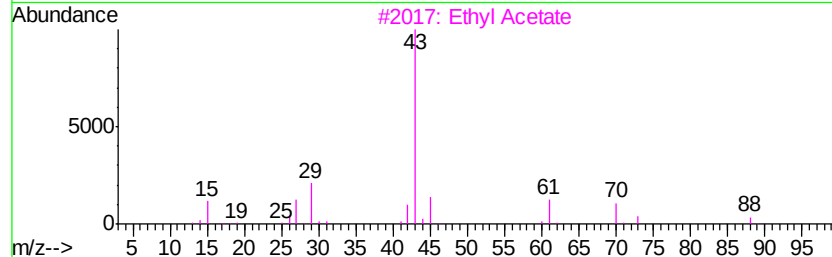
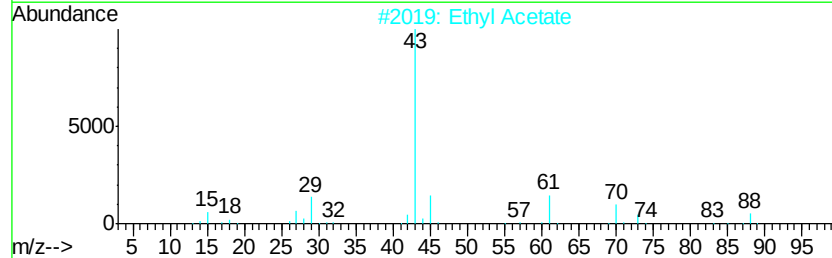
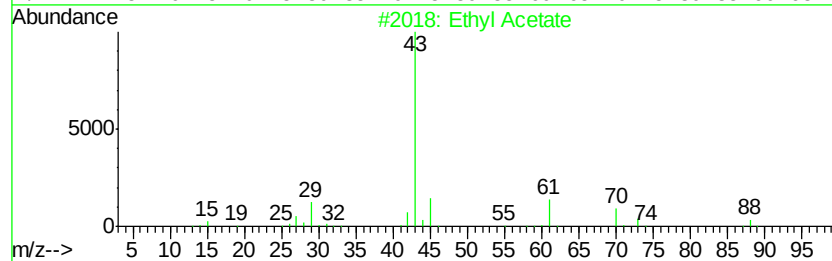
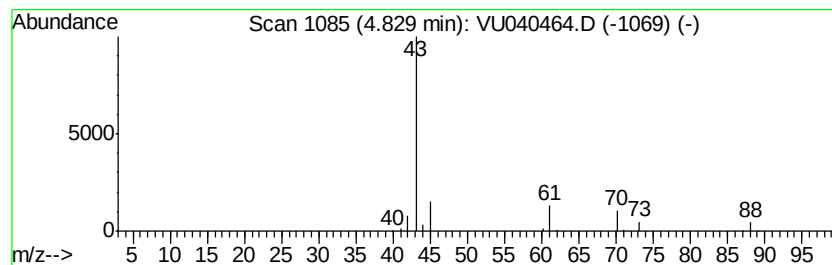
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	3.81 ug/L	249350	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	90
4		Ethyl Acetate	88	C4H8O2	000141-78-6	86
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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ALS Vial : 16 Sample Multiplier: 1

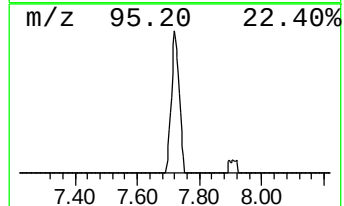
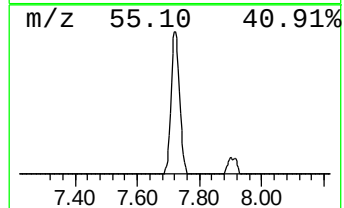
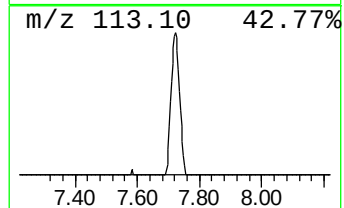
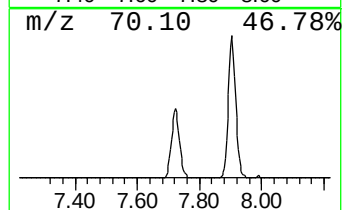
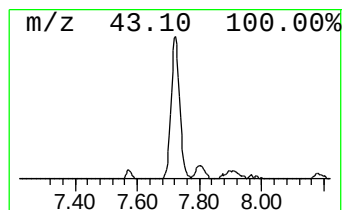
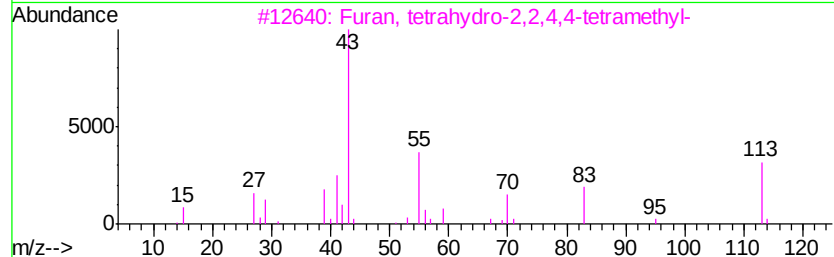
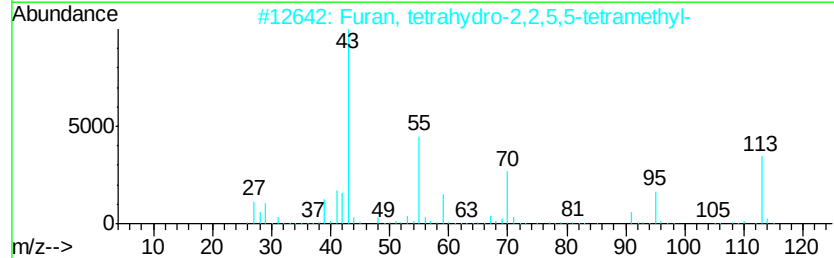
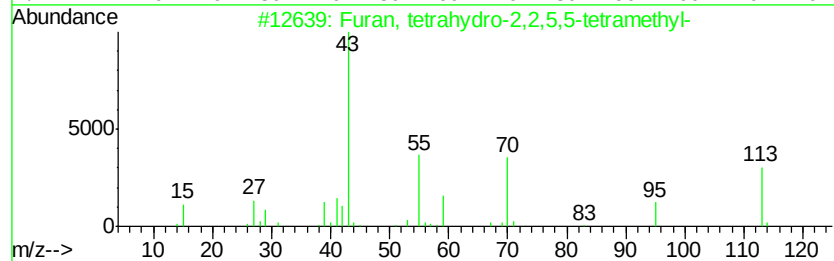
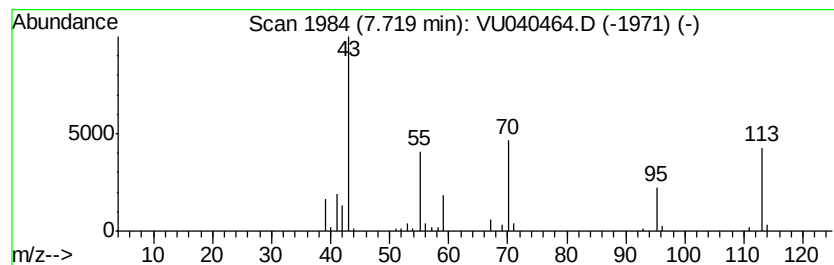
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
7.72	0.77 ug/L	50502	1,4-Difluorobenzene	6.26		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83	
2	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	72	
3	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	47	
4	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	45	
5	2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	42	



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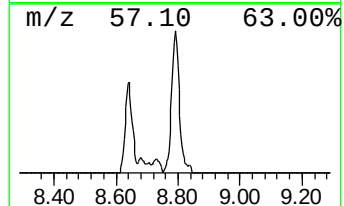
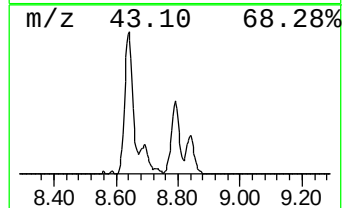
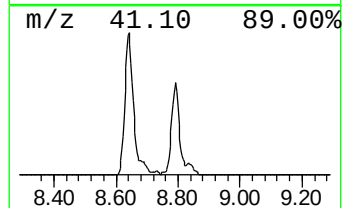
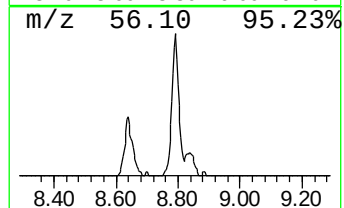
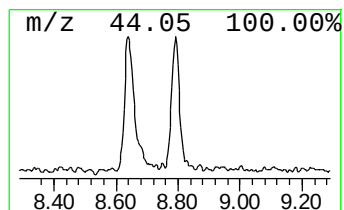
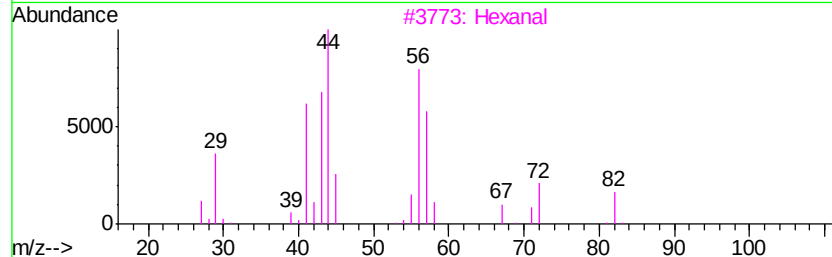
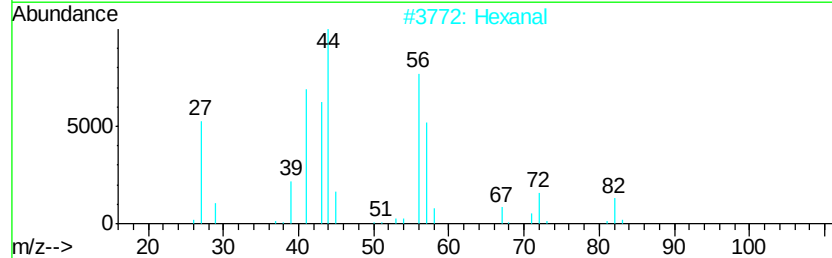
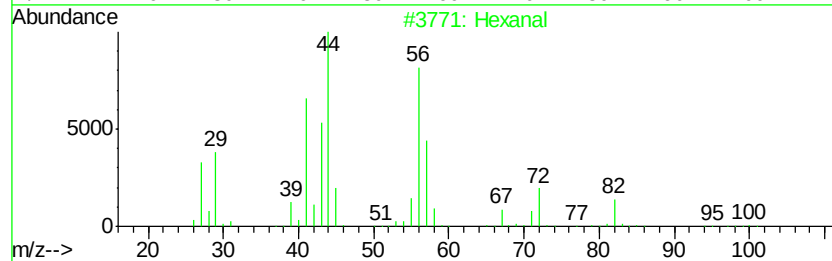
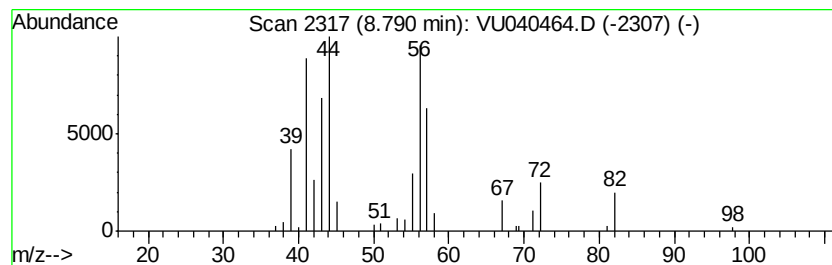
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.79	0.61 ug/L	51159	Chlorobenzene-d5	9.42

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal		100	C6H12O	000066-25-1	64
2	Hexanal		100	C6H12O	000066-25-1	53
3	Hexanal		100	C6H12O	000066-25-1	50
4	Hexanal		100	C6H12O	000066-25-1	45
5	Butanal, 3-methyl-		86	C5H10O	000590-86-3	38



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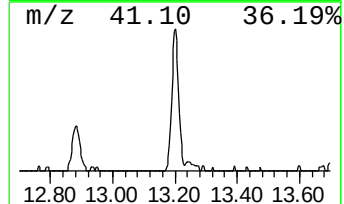
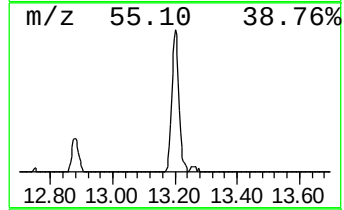
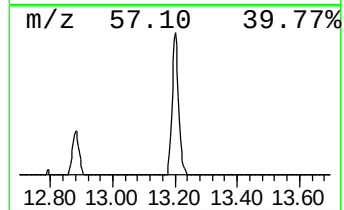
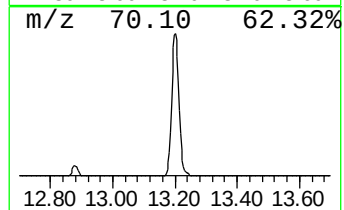
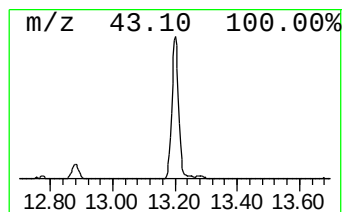
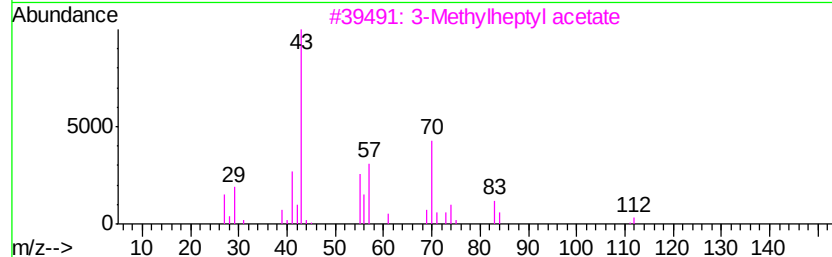
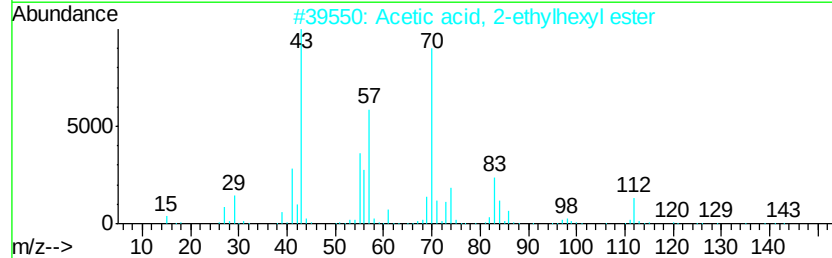
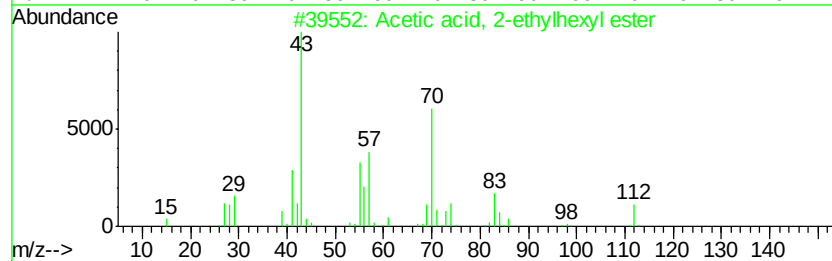
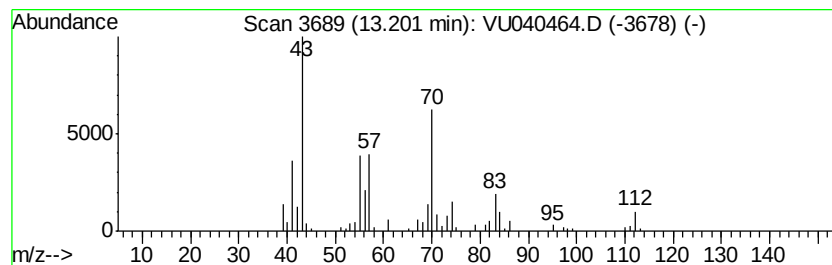
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Acetic acid, 2-ethylhexyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.20	0.89 ug/L	71765	1,4-Dichlorobenzene-d4	11.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	91
2			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	91
3			3-Methylheptyl acetate	172	C10H20O2	072218-58-7	72
4			Carbonic acid, propanoyl 2-ethyl...	212	C12H20O3	1000357-90-9	59
5			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	58



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100220\
Data File : VU040464.D
Acq On : 02 Oct 2020 16:32
Operator : SY/MD
Sample : L4185-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AT2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR092920WMA.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
Propanal, 2-methyl-	3.60	0.8	ug/L	55885	1	6.26	326892	5.0
Ethyl Acetate	4.83	3.8	ug/L	249350	1	6.26	326892	5.0
Furan, tetrahydro...	7.72	0.8	ug/L	50502	1	6.26	326892	5.0
Hexanal	8.79	0.6	ug/L	51159	2	9.42	422010	5.0
Acetic acid, 2-et...	13.20	0.9	ug/L	71765	3	11.81	401803	5.0