

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU021220\
 Data File : VU036731.D
 Acq On : 11 Feb 2020 19:35
 Operator : JC/MD
 Sample : L1414-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AA9

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\SOMUTR021220WMA.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	1.498	38	49	57	rBV2	4471	10588	1.54%	0.172%
2	1.613	75	85	97	rBV	79214	97923	14.25%	1.591%
3	1.700	107	112	120	rVB2	7006	8729	1.27%	0.142%
4	1.932	176	184	197	rVB	64898	82317	11.98%	1.337%
5	2.594	375	390	401	rBV	108002	182930	26.61%	2.972%
6	2.658	401	410	429	rVB	37142	64379	9.37%	1.046%
7	2.793	441	452	469	rBV	26790	50544	7.35%	0.821%
8	3.224	569	586	612	rBV2	156556	352127	51.23%	5.721%
9	4.491	955	980	1003	rBV	214142	558165	81.20%	9.069%
10	4.684	1022	1040	1077	rBV3	108084	327662	47.67%	5.324%
11	4.854	1080	1093	1117	rVB	117254	253113	36.82%	4.113%
12	5.112	1157	1173	1193	rBV	83770	191367	27.84%	3.109%
13	5.430	1259	1272	1288	rVB2	9599	20463	2.98%	0.332%
14	5.767	1351	1377	1401	rBV2	191654	474371	69.01%	7.708%
15	6.288	1523	1539	1558	rBV	162082	303972	44.22%	4.939%
16	6.430	1572	1583	1599	rVB2	7636	14926	2.17%	0.243%
17	6.729	1663	1676	1692	rBV	114367	222660	32.39%	3.618%
18	7.166	1793	1812	1841	rBV	297273	687398	100.00%	11.169%
19	7.600	1935	1947	1967	rBV2	59515	104971	15.27%	1.706%
20	7.931	2034	2050	2066	rBV	235999	407623	59.30%	6.623%
21	8.211	2125	2137	2150	rBV	35911	61875	9.00%	1.005%
22	8.668	2266	2279	2318	rBV	251952	483841	70.39%	7.861%
23	8.819	2318	2326	2339	rVB4	5526	9923	1.44%	0.161%
24	9.446	2508	2521	2553	rBV	219904	368737	53.64%	5.991%
25	10.372	2800	2809	2823	rBV3	5882	9815	1.43%	0.159%
26	10.780	2925	2936	2954	rBV	80406	129956	18.91%	2.112%
27	11.835	3252	3264	3278	rVB	195160	320872	46.68%	5.214%
28	12.214	3370	3382	3397	rBV	199421	321218	46.73%	5.219%
29	12.526	3469	3479	3492	rVB2	7295	11726	1.71%	0.191%
30	14.333	4031	4041	4052	rBV3	13241	20377	2.96%	0.331%

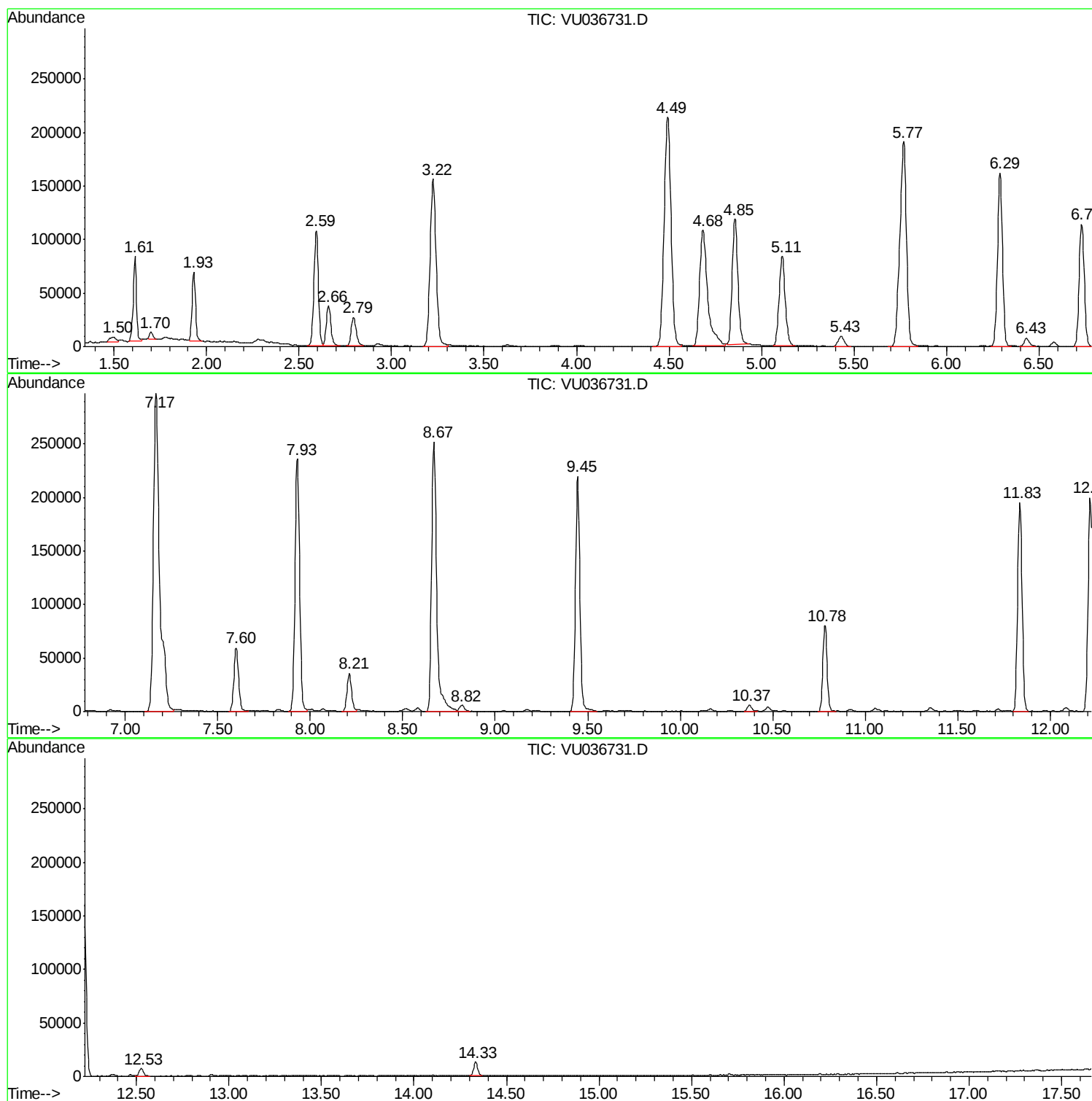
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AA9

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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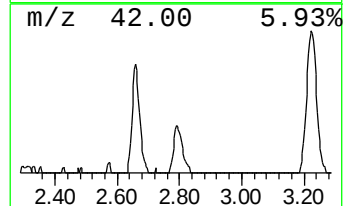
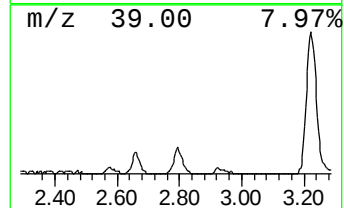
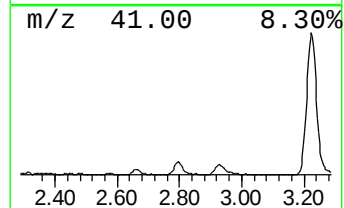
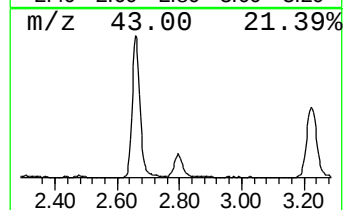
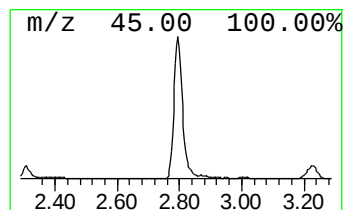
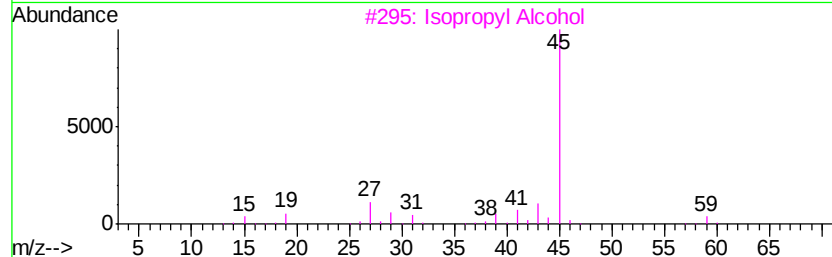
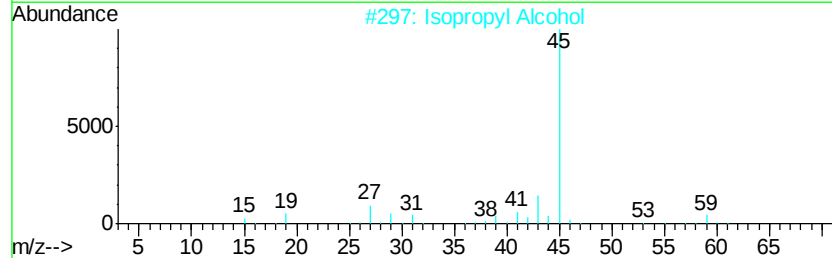
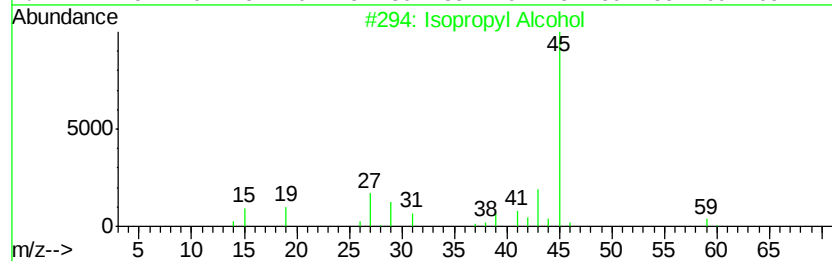
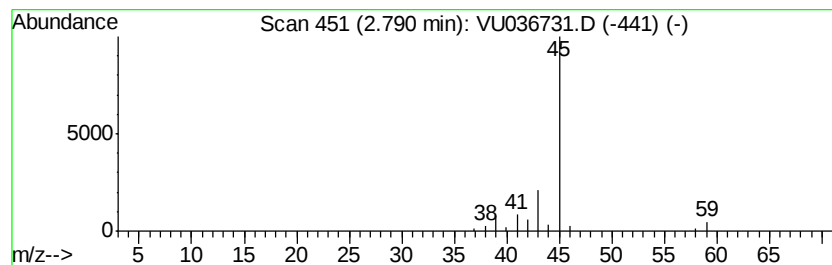
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	0.83 ug/L	50544	1,4-Difluorobenzene	6.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Ethylamine	45	C2H7N	000075-04-7	5
5			2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4



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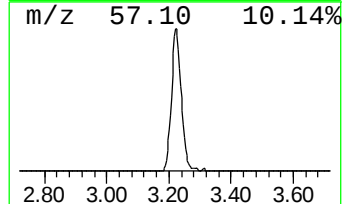
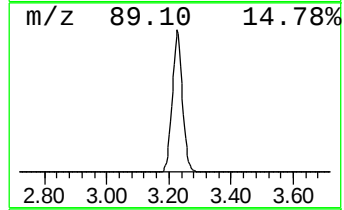
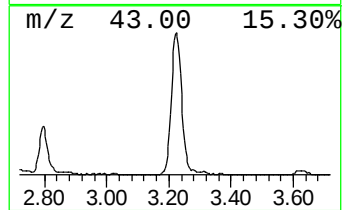
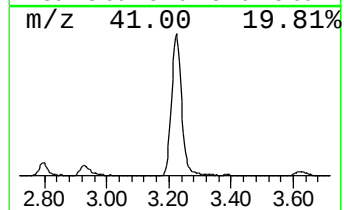
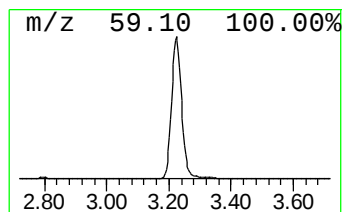
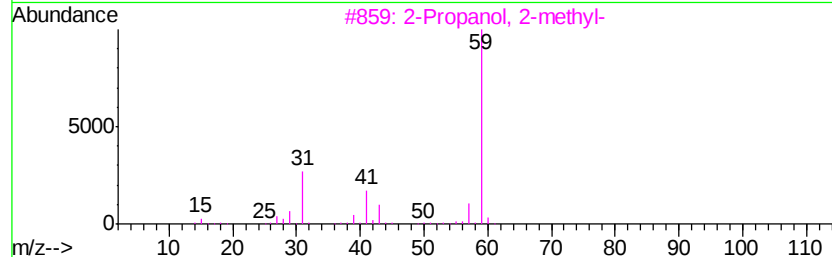
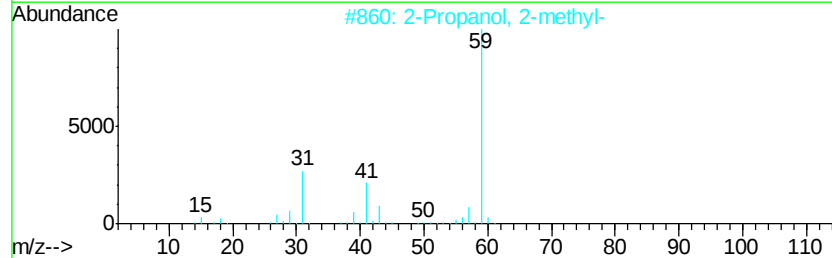
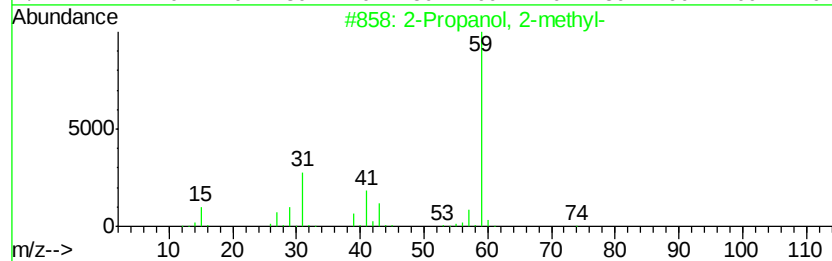
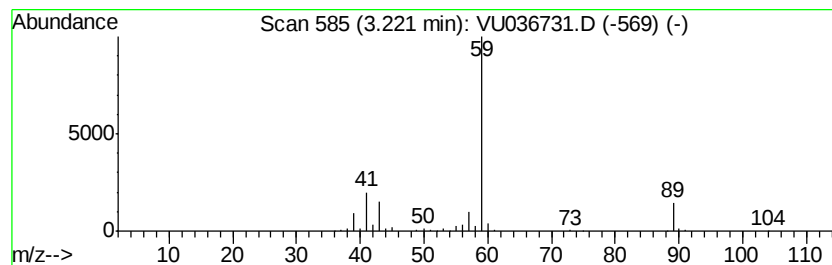
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR021220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	5.79 ug/L	352127	1,4-Difluorobenzene	6.29

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
2			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	50
3			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39
4			1,2-Butanediol	90	C4H10O2	000584-03-2	38
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	36



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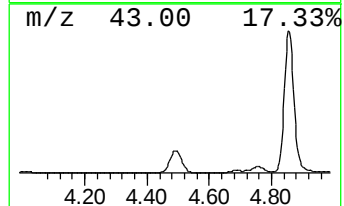
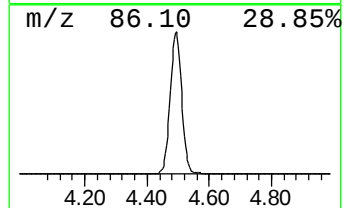
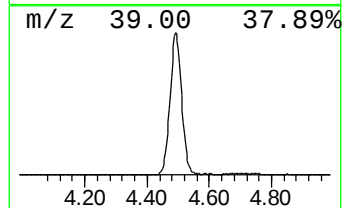
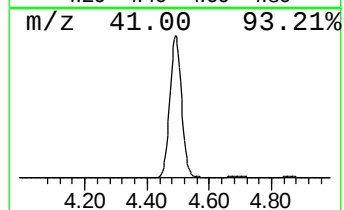
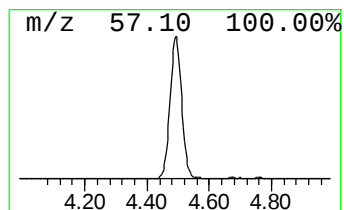
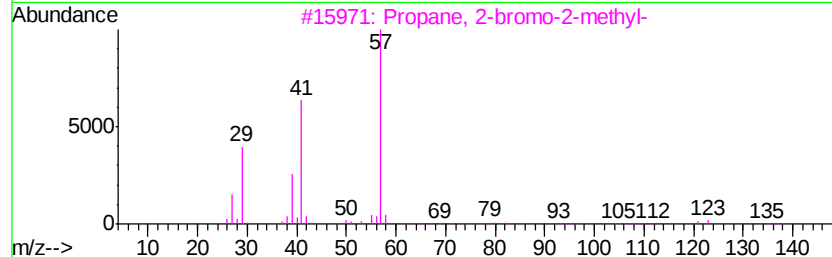
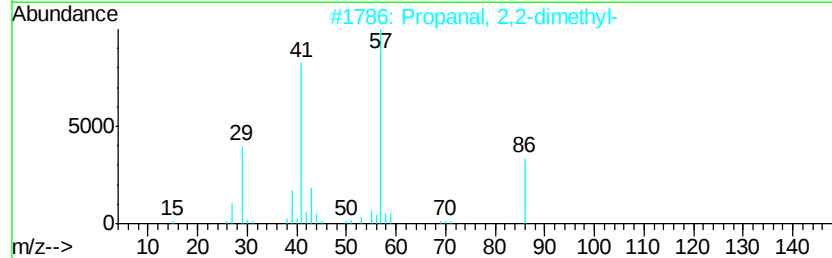
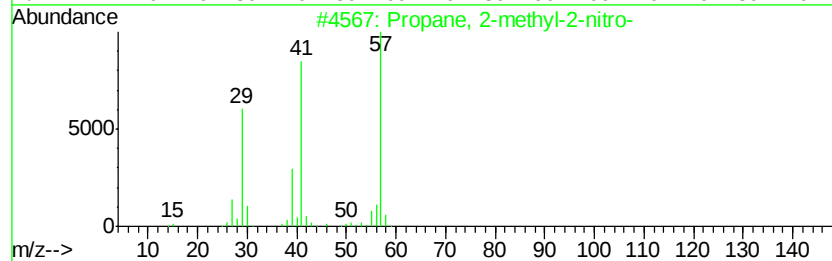
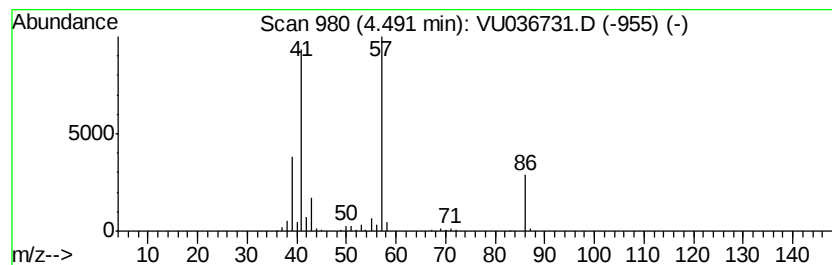
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Propane, 2-methyl-2-nitro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.49	9.18 ug/L	558165	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
2		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	47
3		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	45
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	45
5		3-Pentanone	86	C5H10O	000096-22-0	42



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ALS Vial : 10 Sample Multiplier: 1

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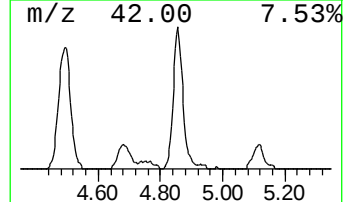
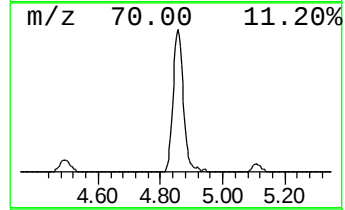
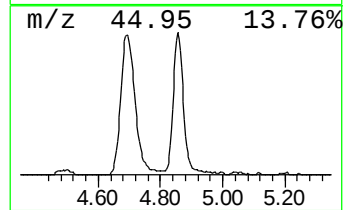
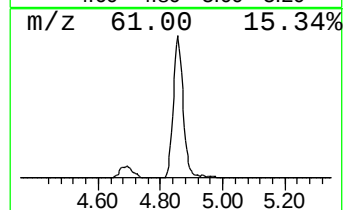
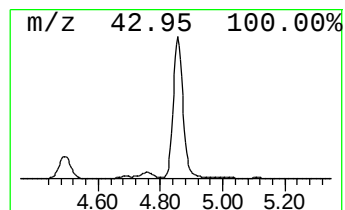
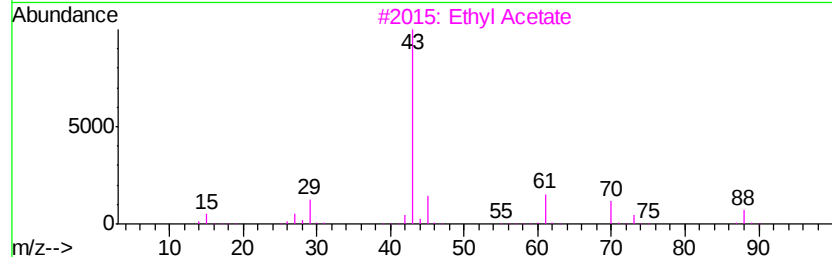
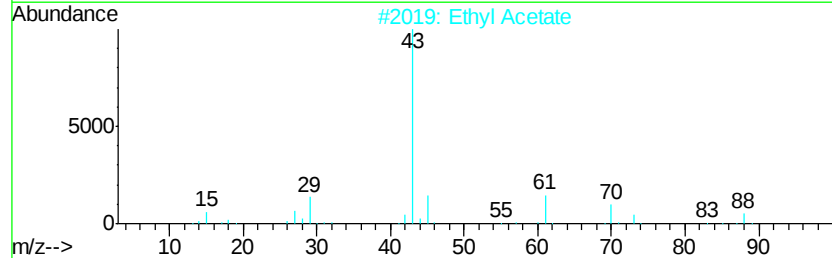
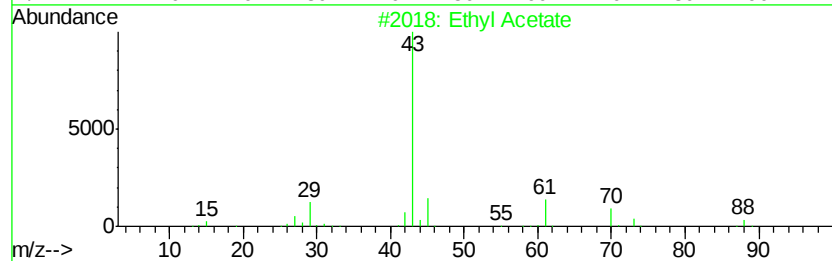
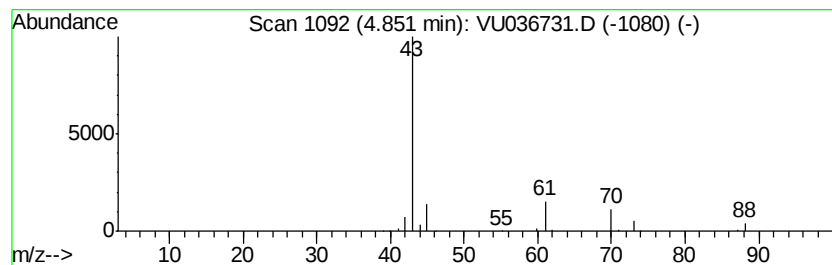
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethyl Acetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	4.16 ug/L	253113	1,4-Difluorobenzene	6.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	86
2		Ethyl Acetate	88	C4H8O2	000141-78-6	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	78
4		Ethyl Acetate	88	C4H8O2	000141-78-6	72
5		(3-Methyl-oxiran-2-yl)-methanol	88	C4H8O2	1000194-22-9	9



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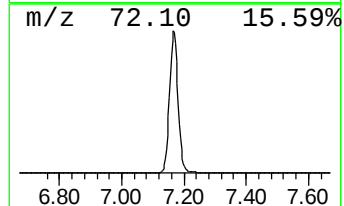
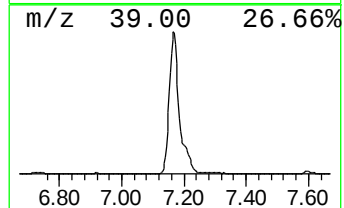
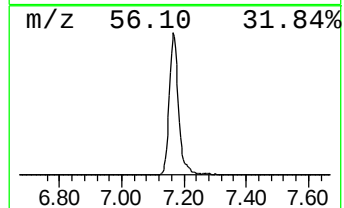
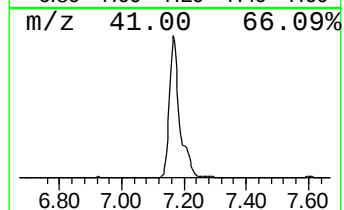
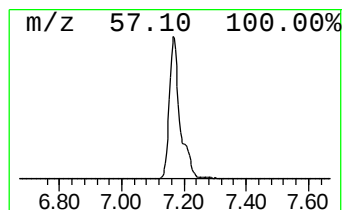
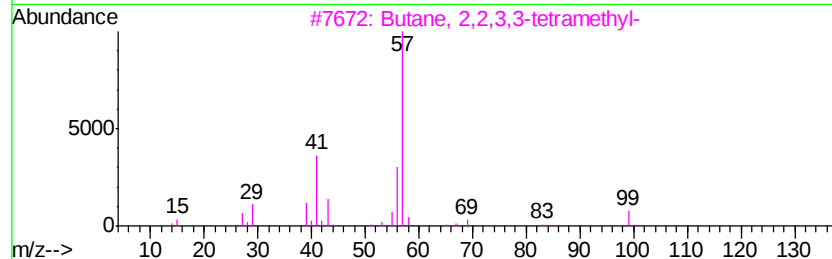
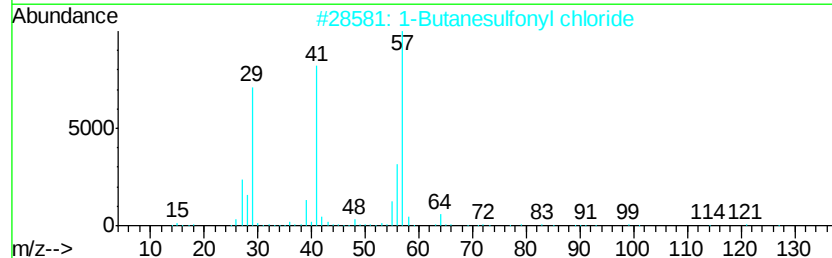
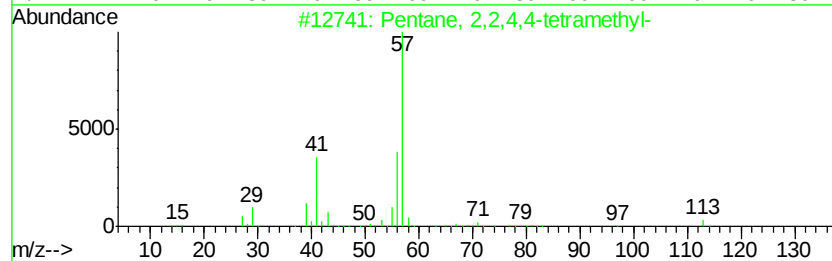
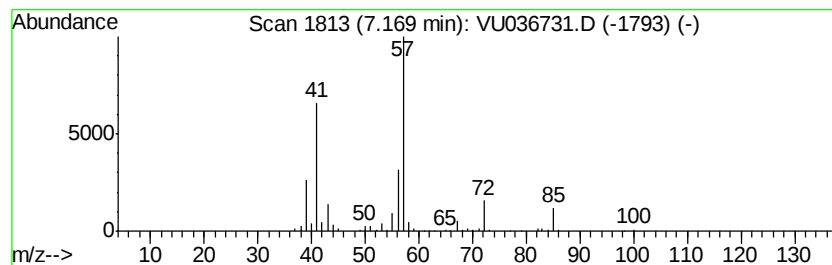
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TIC Library : C:\DATABASE\NIST11.L
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 Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.17	11.31 ug/L	687398	1,4-Difluorobenzene	6.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	40
2		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	40
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	40
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
5		Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.79	0.8	ug/L	50544	1	6.29	303972	5.0
2-Propanol, 2-met...	3.22	5.8	ug/L	352127	1	6.29	303972	5.0
Propane, 2-methyl...	4.49	9.2	ug/L	558165	1	6.29	303972	5.0
Ethyl Acetate	4.85	4.2	ug/L	253113	1	6.29	303972	5.0
(DEL) Alkane: Str...	7.17	11.3	ug/L	687398	1	6.29	303972	5.0