

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
 Data File : VU040084.D
 Acq On : 10 Sep 2020 16:27
 Operator : SY/MD
 Sample : L3961-01
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4Y25

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	1.495	42	48	56	rBV	11226	11624	2.59%	0.260%
2	1.604	71	82	92	rVB	53170	67051	14.95%	1.499%
3	1.922	172	181	191	rVB	40864	52226	11.64%	1.167%
4	2.581	372	386	398	rBV2	85776	141462	31.54%	3.162%
5	2.652	398	408	433	rVB	33138	75812	16.90%	1.694%
6	2.829	440	463	517	rBV2	64045	367398	81.92%	8.211%
7	3.379	620	634	654	rVB2	26371	62477	13.93%	1.396%
8	3.893	782	794	804	rVB3	3593	7345	1.64%	0.164%
9	4.012	817	831	847	rVB4	3565	9070	2.02%	0.203%
10	4.520	972	989	1013	rBV2	38574	95919	21.39%	2.144%
11	4.649	1014	1029	1050	rBV	68678	179131	39.94%	4.004%
12	4.826	1070	1084	1099	rVB2	16507	36326	8.10%	0.812%
13	5.083	1147	1164	1179	rBV2	74613	164319	36.64%	3.673%
14	5.597	1309	1324	1341	rBV3	17371	38931	8.68%	0.870%
15	5.742	1348	1369	1387	rBV2	141805	370372	82.58%	8.278%
16	6.263	1517	1531	1551	rBV2	161398	308399	68.76%	6.893%
17	6.510	1594	1608	1623	rBV2	24077	49219	10.97%	1.100%
18	6.703	1648	1668	1682	rBV2	92362	178652	39.83%	3.993%
19	7.166	1800	1812	1822	rBV4	7572	13948	3.11%	0.312%
20	7.227	1822	1831	1844	rVB8	5927	10429	2.33%	0.233%
21	7.308	1844	1856	1870	rBV3	13890	24756	5.52%	0.553%
22	7.498	1909	1915	1925	rVB6	4050	7429	1.66%	0.166%
23	7.575	1928	1939	1954	rVB3	46107	81180	18.10%	1.814%
24	7.726	1973	1986	1997	rVB4	8362	16222	3.62%	0.363%
25	7.906	2014	2042	2055	rBV	167787	315653	70.38%	7.055%
26	8.186	2116	2129	2146	rBV	29618	52462	11.70%	1.173%
27	8.510	2219	2230	2239	rVB6	5879	9959	2.22%	0.223%
28	8.639	2257	2270	2300	rBV	252967	448494	100.00%	10.024%
29	8.925	2349	2359	2372	rBV3	6057	12385	2.76%	0.277%
30	9.420	2500	2513	2531	rBV	241333	401794	89.59%	8.980%
31	10.755	2914	2928	2950	rVB3	70344	118716	26.47%	2.653%
32	11.472	3140	3151	3174	rVB2	32711	53075	11.83%	1.186%
33	11.806	3243	3255	3270	rBV	238158	386208	86.11%	8.632%
34	12.057	3323	3333	3346	rBV2	17977	29842	6.65%	0.667%

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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\SOMUTR083120WMA.M
Title : TRACE VOA SOM01.0

35	12.189	3362	3374	3388	rBV	172492	275932	61.52%	6.167%
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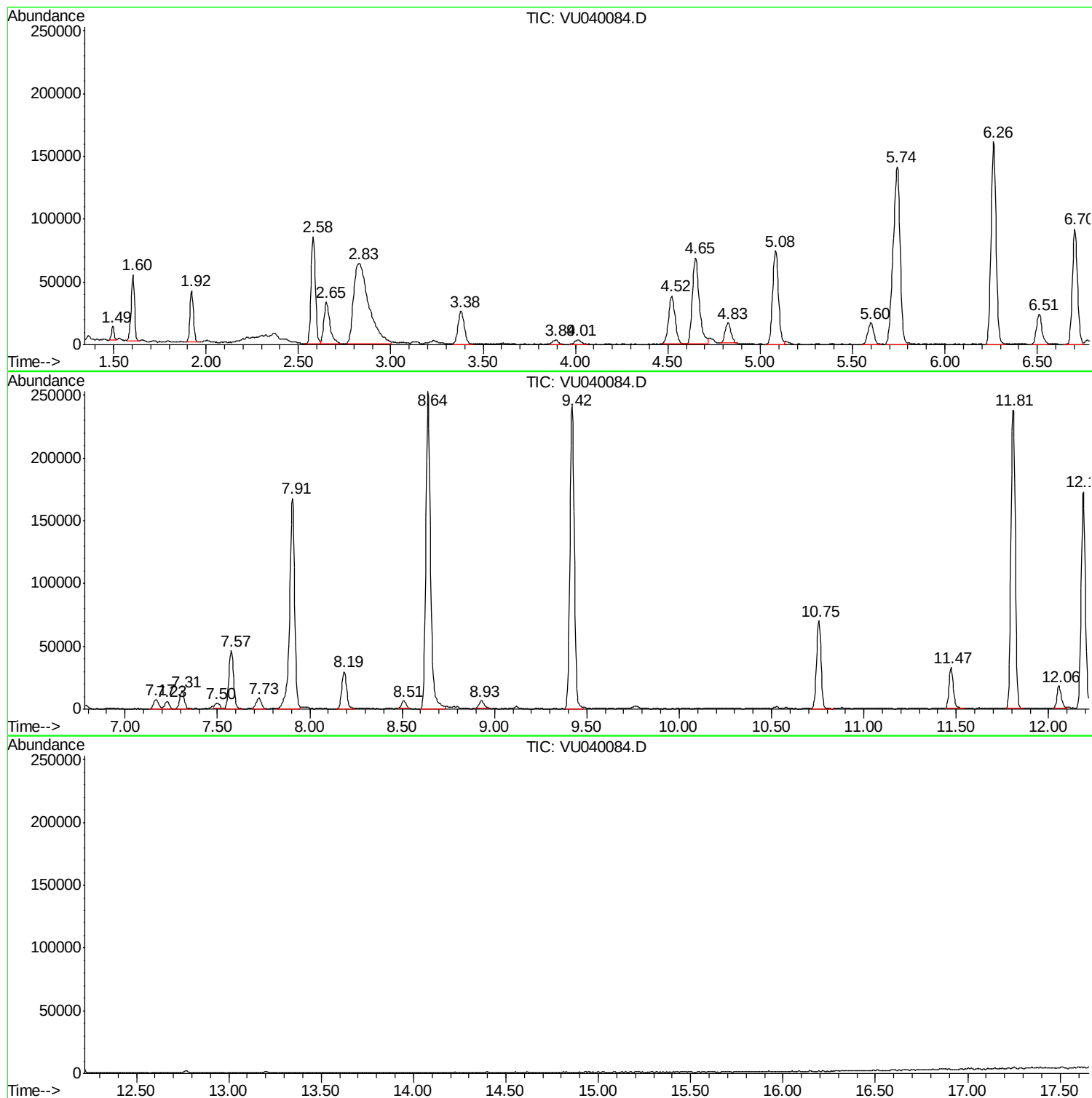
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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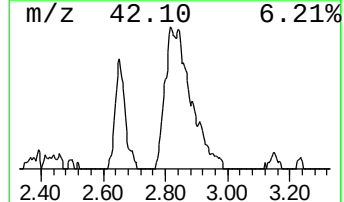
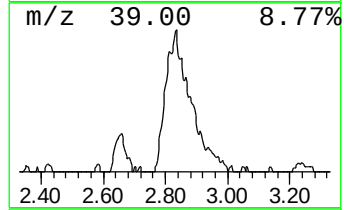
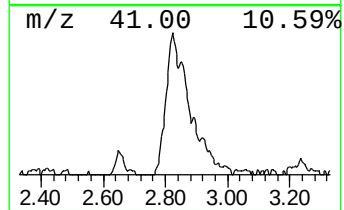
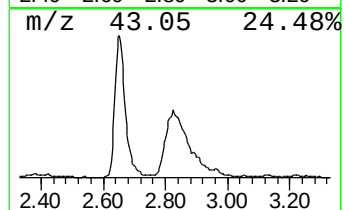
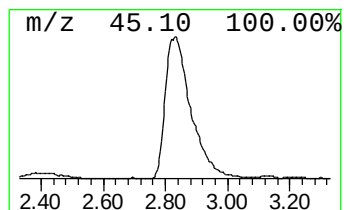
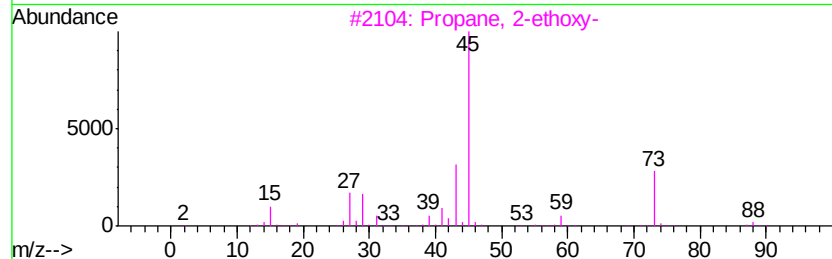
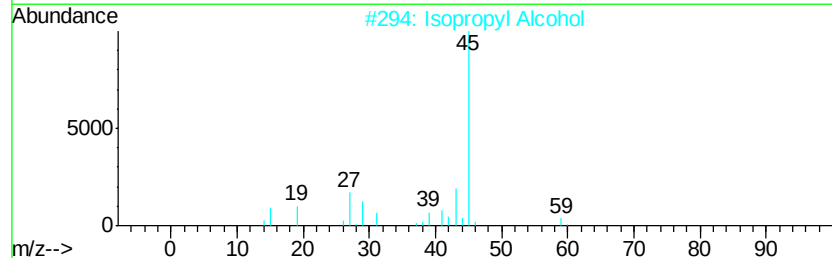
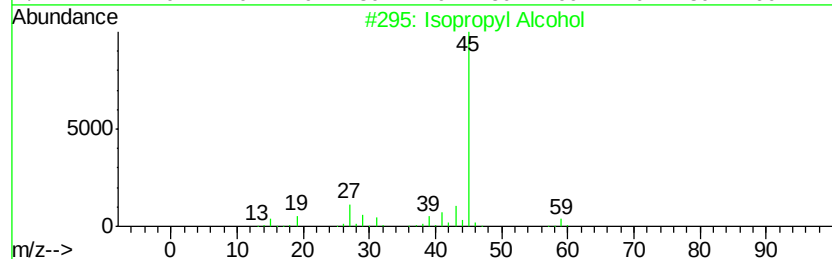
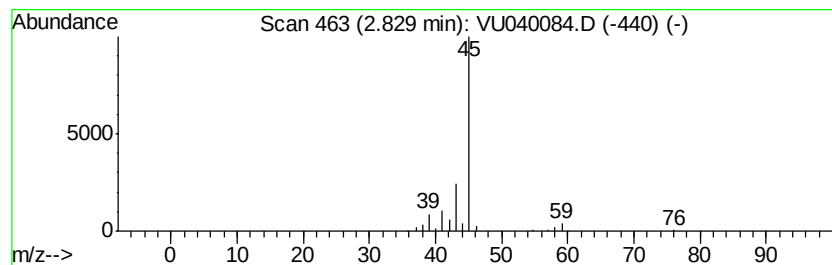
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	5.96 ug/L	367398	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
4		Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40



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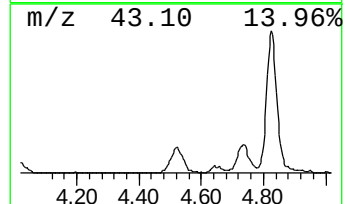
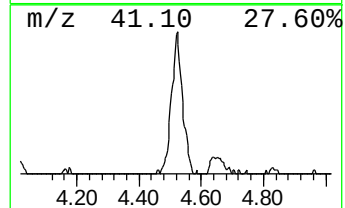
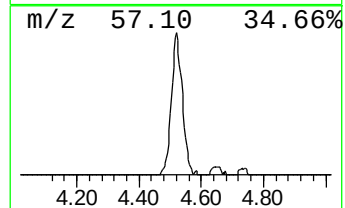
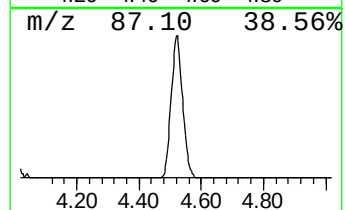
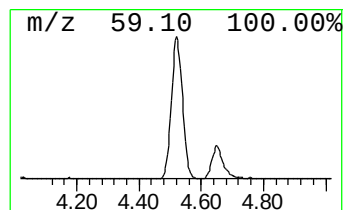
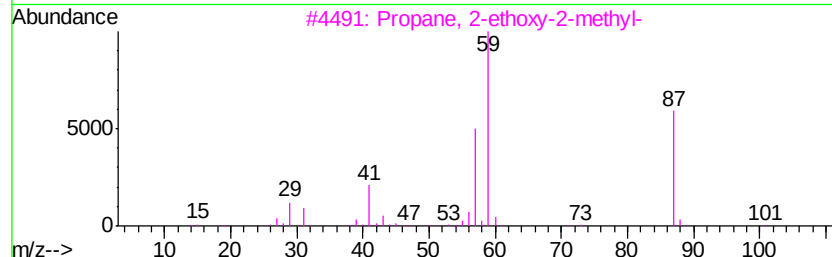
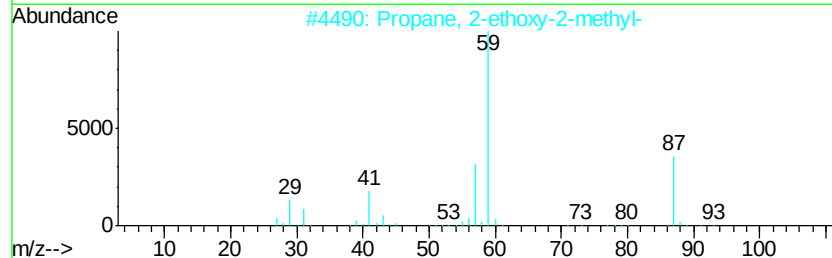
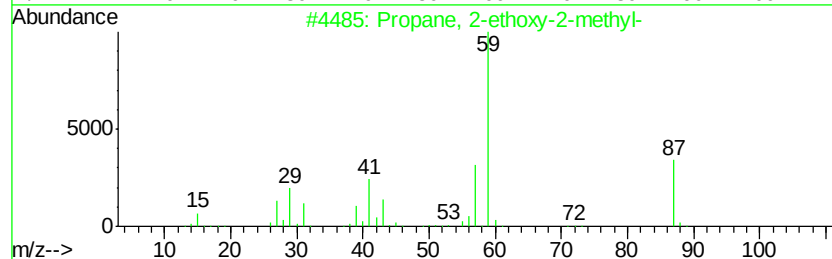
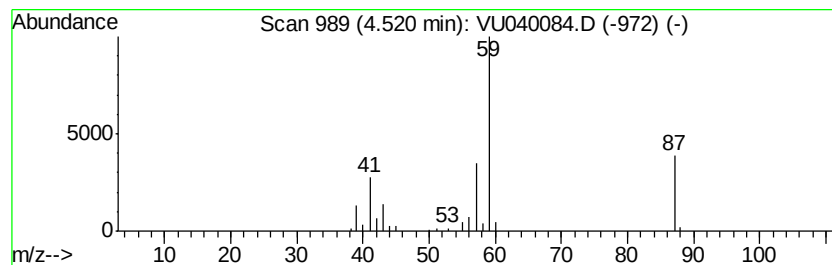
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	1.56 ug/L	95919	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	83
2		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	78
3		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	74
4		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	40



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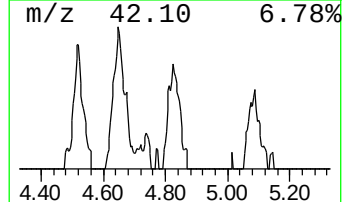
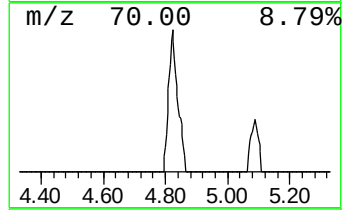
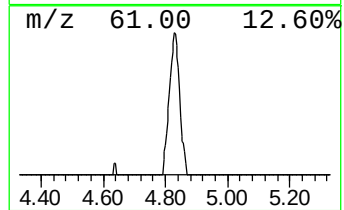
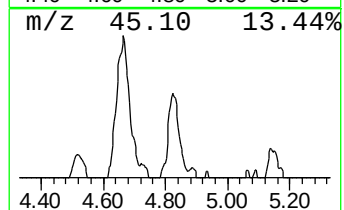
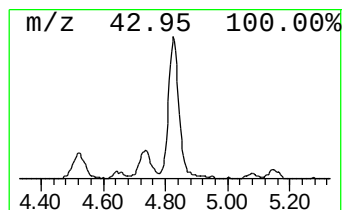
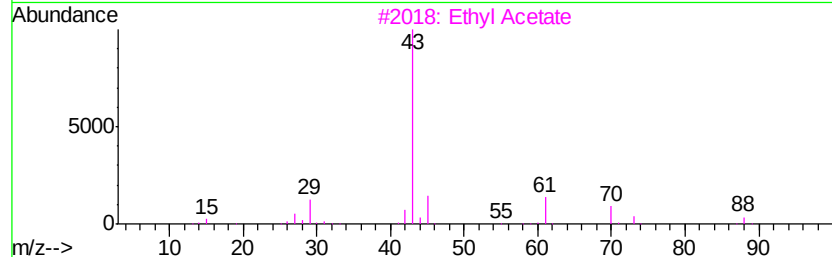
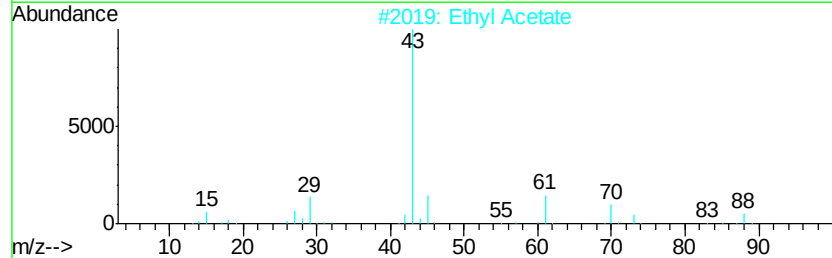
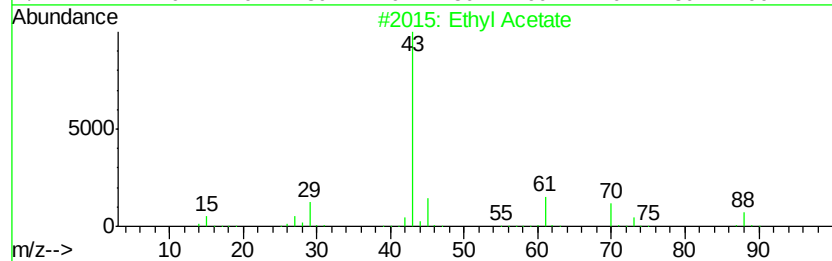
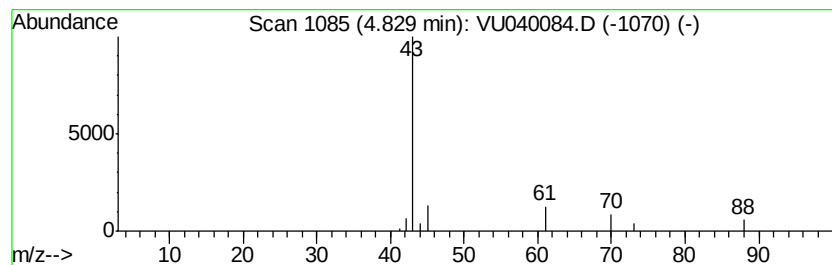
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Ethyl Acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.59 ug/L	36326	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	74
4	Ethyl Acetate		88	C4H8O2	000141-78-6	74
5	CH3C(O)CH2CH2OH		88	C4H8O2	000590-90-9	38



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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

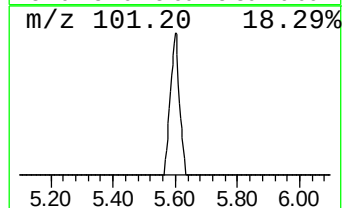
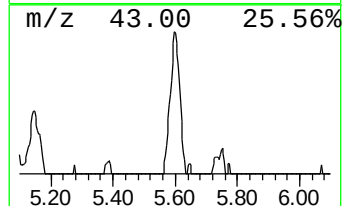
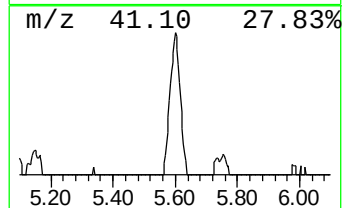
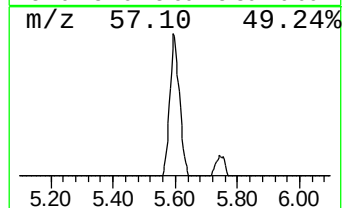
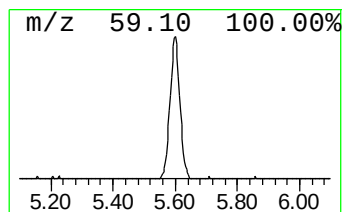
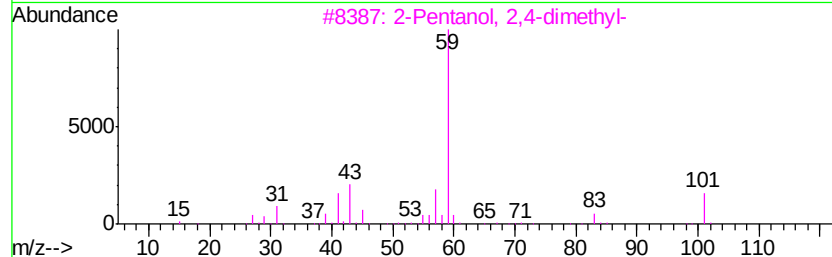
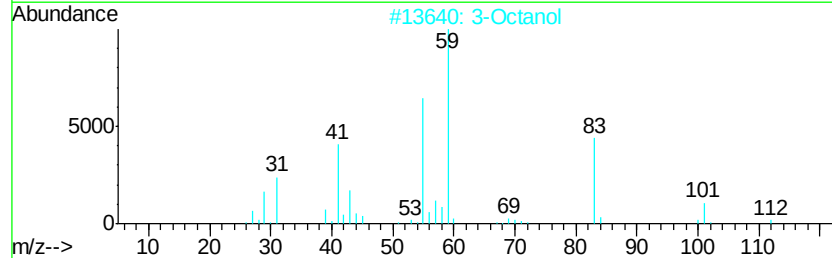
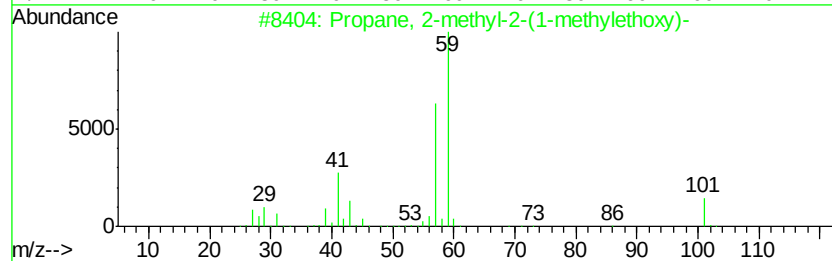
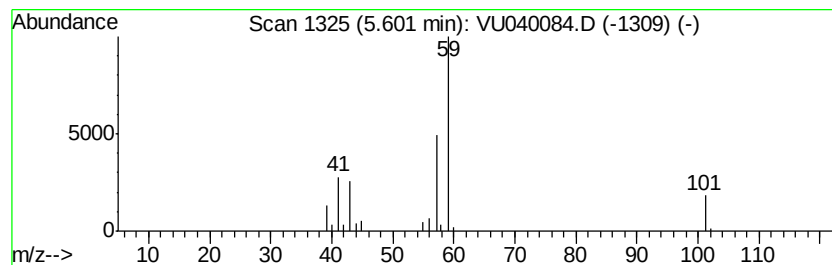
Instrument :
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ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Propane, 2-methyl-2-(1-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.60	0.63 ug/L	38931	1,4-Difluorobenzene	6.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	74
2	3-Octanol	130	C8H18O	000589-98-0	43
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	43
4	Butanoic acid, 3,3-dimethyl-	116	C6H12O2	001070-83-3	39
5	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9



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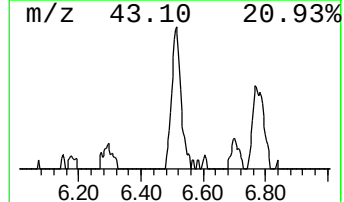
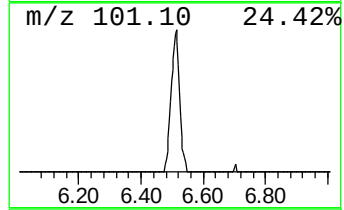
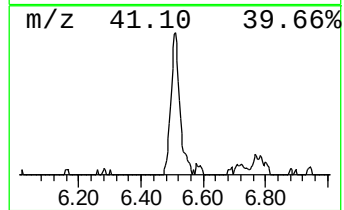
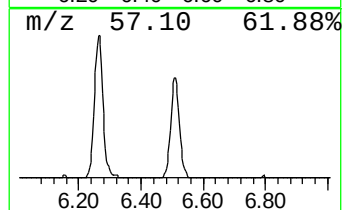
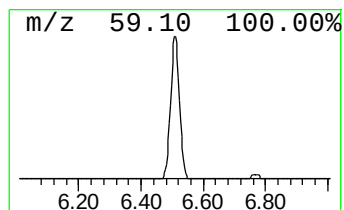
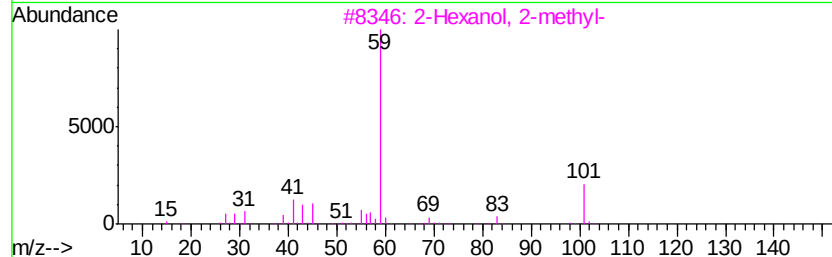
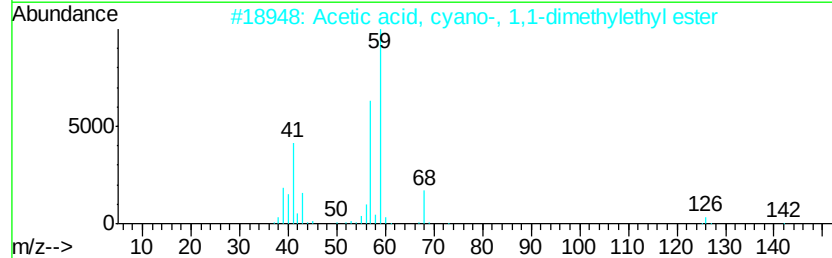
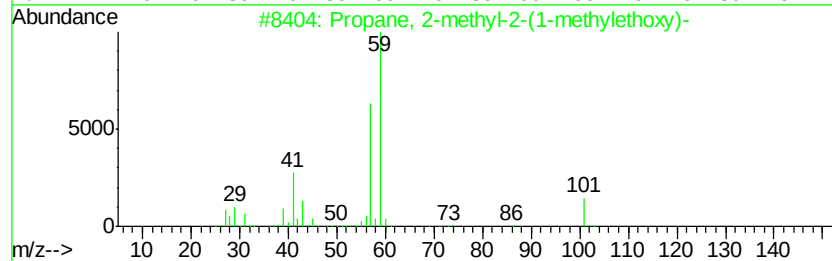
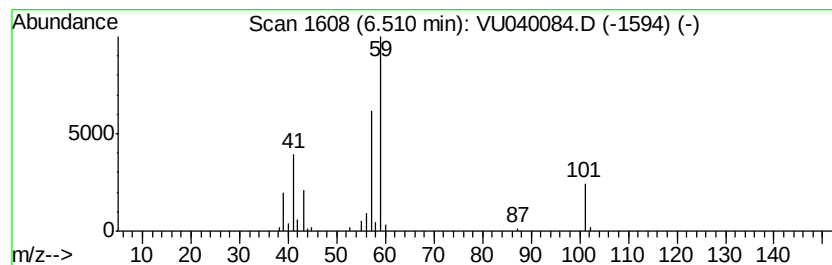
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Acetic acid, cyano-, 1,1-di... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	0.80 ug/L	49219	1,4-Difluorobenzene	6.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	74	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	64	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40	
4	3-Octanol	130	C8H18O	000589-98-0	40	
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40	



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Operator : SY/MD
Sample : L3961-01
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y25

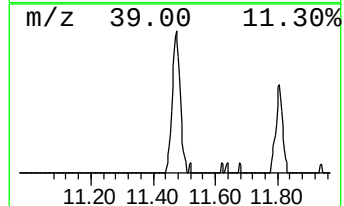
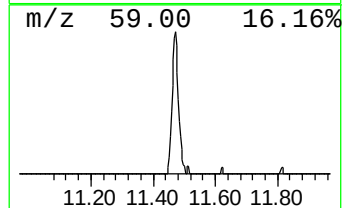
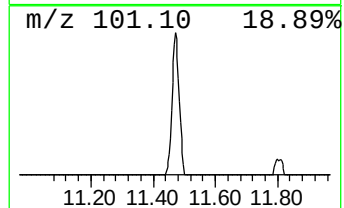
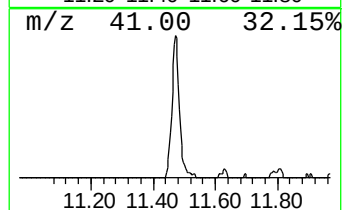
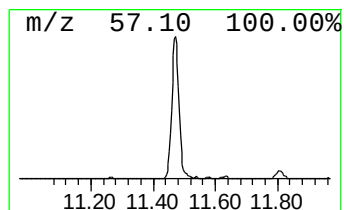
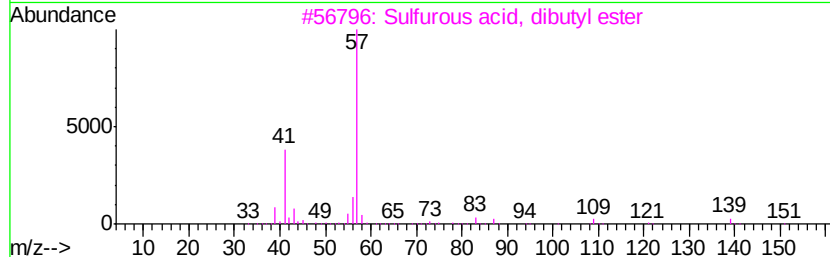
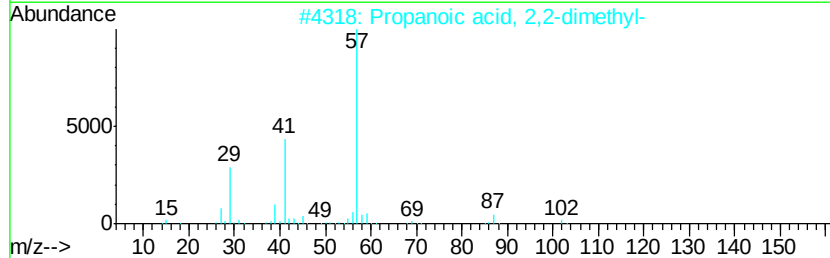
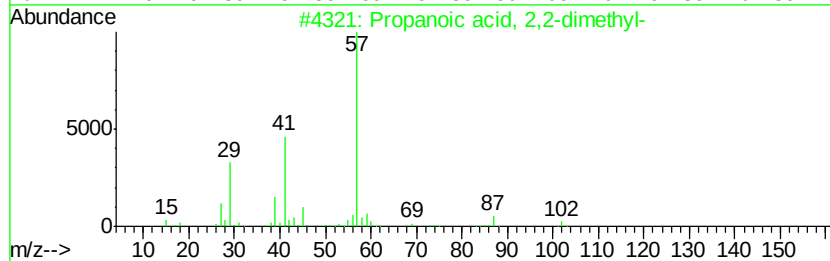
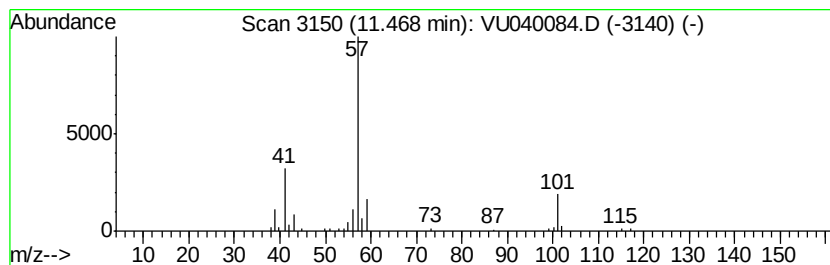
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.69 ug/L	53075	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	43
2		Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	37
3		Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	35
4		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	32
5		Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	32



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091020\
Data File : VU040084.D
Acq On : 10 Sep 2020 16:27
Operator : SY/MD
Sample : L3961-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y25

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.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
Isopropyl Alcohol	2.83	6.0	ug/L	367398	1	6.26	308399	5.0
Propane, 2-ethoxy...	4.52	1.6	ug/L	95919	1	6.26	308399	5.0
Ethyl Acetate	4.83	0.6	ug/L	36326	1	6.26	308399	5.0
Propane, 2-methyl...	5.60	0.6	ug/L	38931	1	6.26	308399	5.0
Acetic acid, cyan...	6.51	0.8	ug/L	49219	1	6.26	308399	5.0
unknown-01	11.47	0.7	ug/L	53075	3	11.81	386208	5.0