

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
 Data File : VU040086.D
 Acq On : 10 Sep 2020 17:14
 Operator : SY/MD
 Sample : L3961-03
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4Y27

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	55	rBV	11122	10825	2.49%	0.245%
2	1.604	71	82	94	rVB2	50739	67345	15.46%	1.523%
3	1.922	172	181	189	rBV	37543	47411	10.88%	1.072%
4	2.006	195	207	209	rBV6	8087	13124	3.01%	0.297%
5	2.578	374	385	397	rBV	80549	132065	30.32%	2.986%
6	2.652	397	408	430	rVB	31429	74302	17.06%	1.680%
7	2.826	438	462	520	rBV	75985	435603	100.00%	9.850%
8	3.379	620	634	651	rBV3	26741	62437	14.33%	1.412%
9	3.887	780	792	805	rBV2	4071	8937	2.05%	0.202%
10	4.009	814	830	832	rBV4	3659	4988	1.15%	0.113%
11	4.520	971	989	1006	rBV2	38167	97446	22.37%	2.203%
12	4.649	1011	1029	1050	rBV2	63503	169013	38.80%	3.822%
13	4.826	1072	1084	1103	rVB	19175	43393	9.96%	0.981%
14	5.083	1148	1164	1180	rBV2	69237	154610	35.49%	3.496%
15	5.601	1309	1325	1340	rBV3	17387	40256	9.24%	0.910%
16	5.742	1348	1369	1385	rBV3	134251	349377	80.21%	7.900%
17	6.263	1512	1531	1551	rBV	160622	301526	69.22%	6.818%
18	6.510	1591	1608	1626	rBV4	25101	52906	12.15%	1.196%
19	6.703	1654	1668	1683	rBV	87211	167920	38.55%	3.797%
20	7.170	1802	1813	1821	rBV4	7879	14116	3.24%	0.319%
21	7.224	1821	1830	1842	rVV4	6489	11409	2.62%	0.258%
22	7.305	1844	1855	1872	rVB5	13087	24376	5.60%	0.551%
23	7.498	1910	1915	1927	rVB4	4709	7312	1.68%	0.165%
24	7.575	1927	1939	1952	rBV2	43546	76249	17.50%	1.724%
25	7.726	1974	1986	1999	rVB6	8347	15827	3.63%	0.358%
26	7.906	2016	2042	2057	rBV	159477	305758	70.19%	6.914%
27	8.186	2119	2129	2144	rBV2	27540	45896	10.54%	1.038%
28	8.510	2218	2230	2241	rVB5	6165	12035	2.76%	0.272%
29	8.639	2258	2270	2293	rBV	237266	422354	96.96%	9.550%
30	8.932	2350	2361	2373	rBV3	6294	13500	3.10%	0.305%
31	9.420	2495	2513	2539	rBV	236454	393300	90.29%	8.893%
32	9.761	2609	2619	2634	rVB8	3140	7218	1.66%	0.163%
33	10.755	2913	2928	2945	rVB2	68287	111814	25.67%	2.528%
34	11.472	3137	3151	3164	rBV	32911	52368	12.02%	1.184%

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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	11.806	3243	3255	3273	rBV	230538	365761	83.97%	8.271%
36	12.054	3322	3332	3347	rBV2	26822	45499	10.45%	1.029%
37	12.189	3362	3374	3389	rVB	162149	264165	60.64%	5.973%

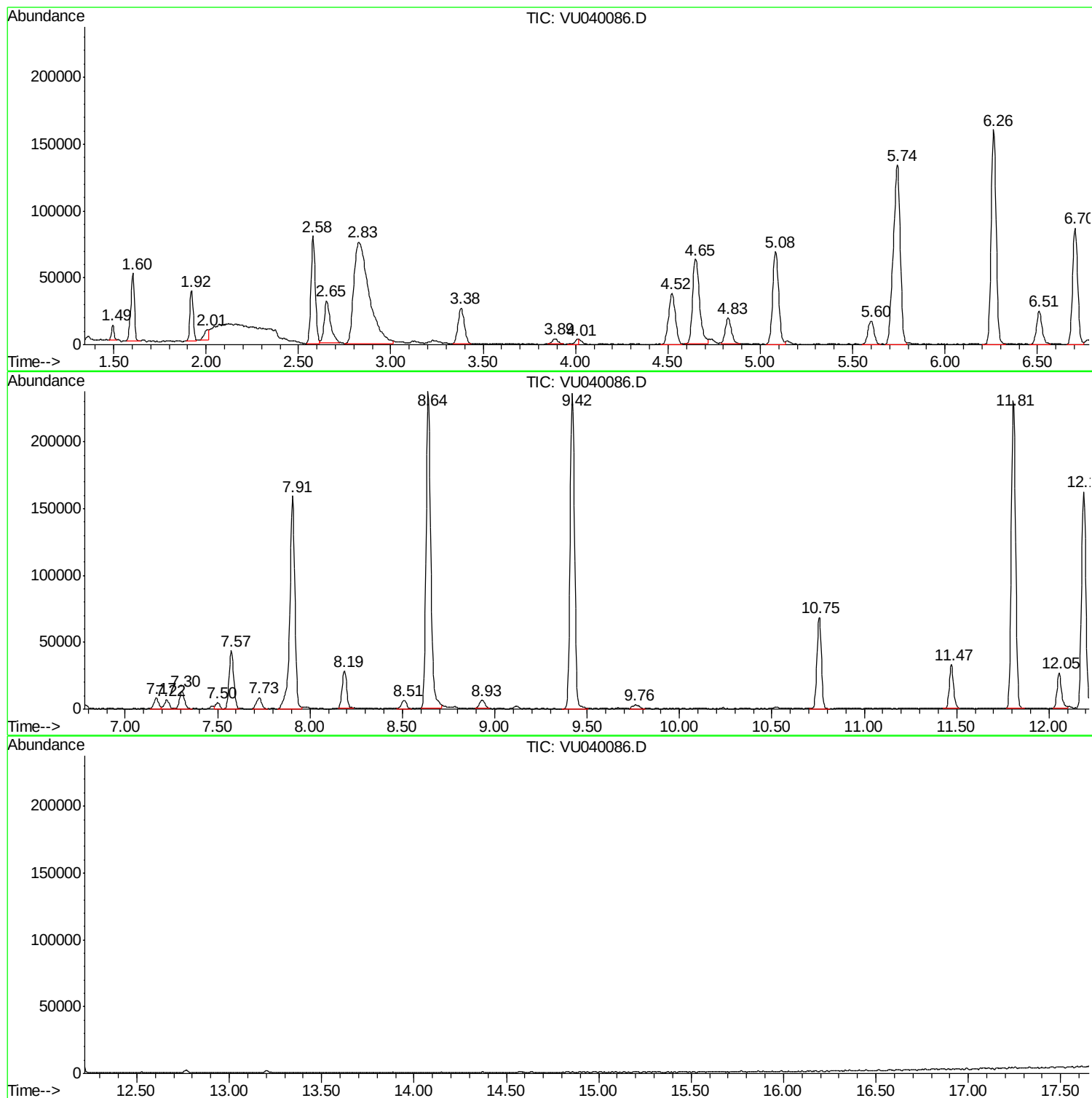
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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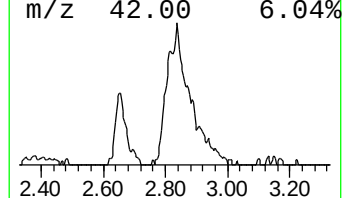
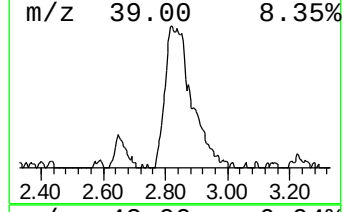
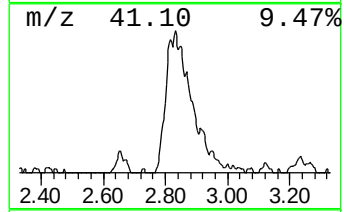
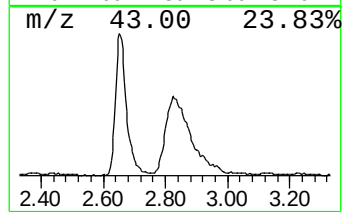
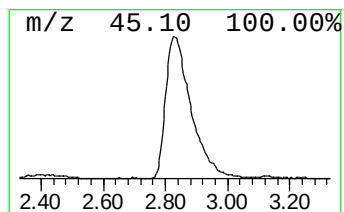
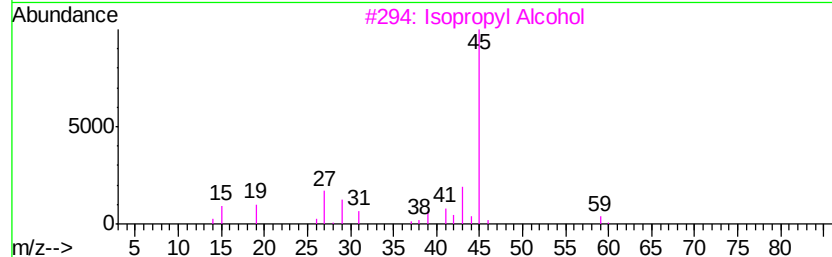
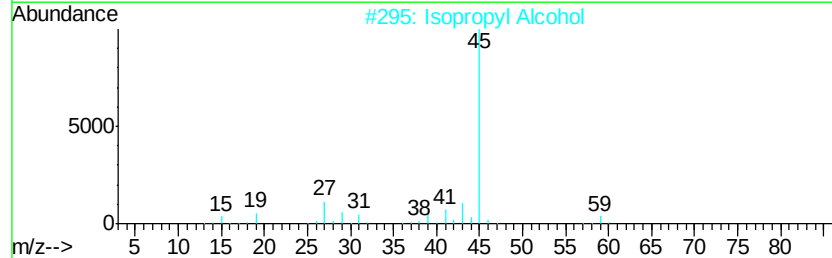
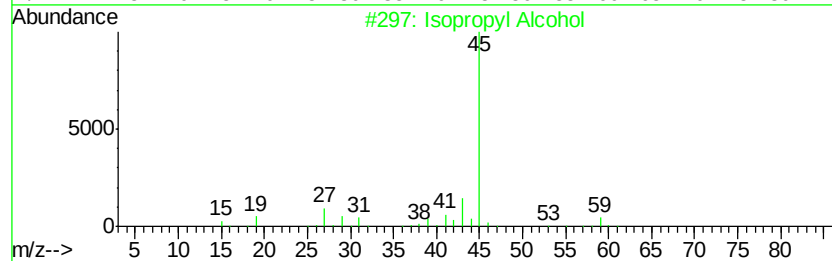
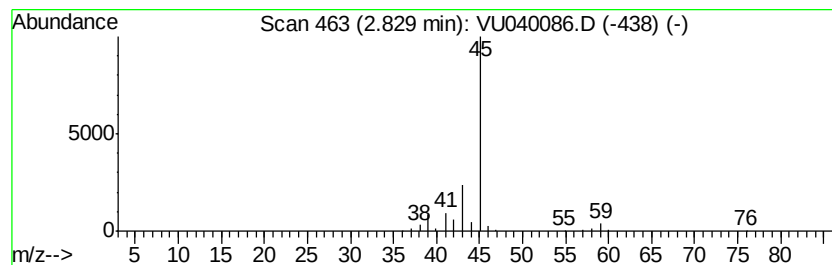
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Quant Title : TRACE VOA SOM01.0

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	7.22 ug/L	435603	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
4		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56
5		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56



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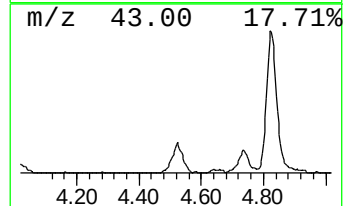
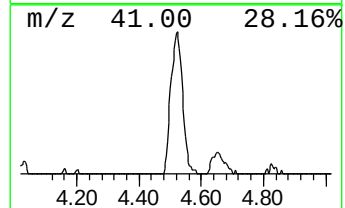
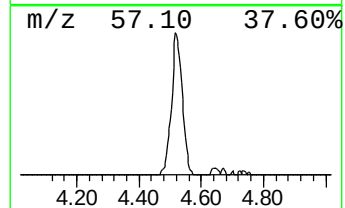
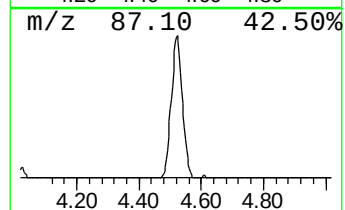
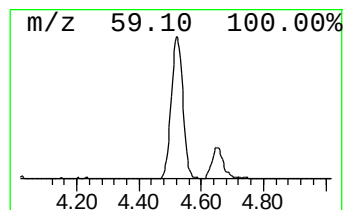
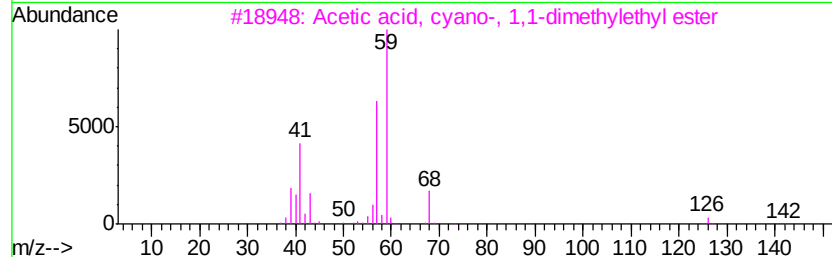
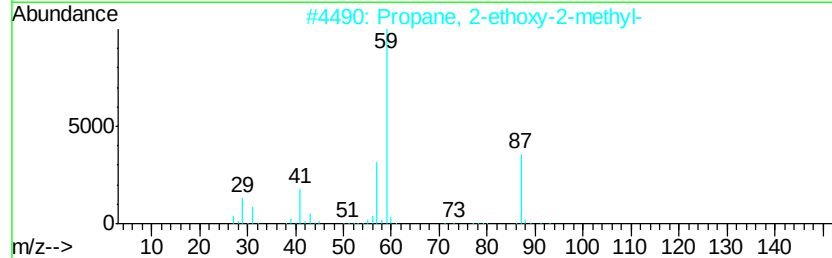
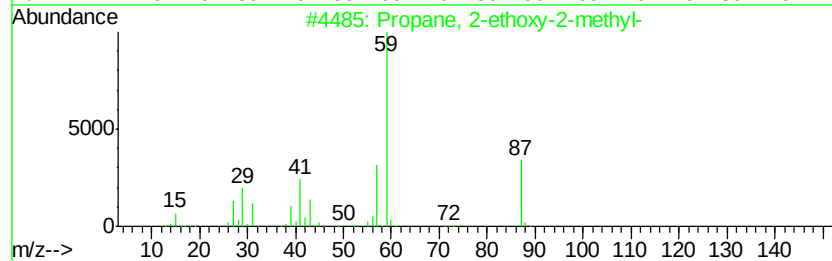
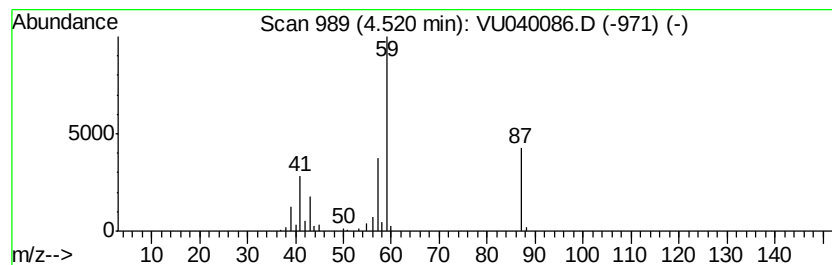
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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	1.62 ug/L	97446	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		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	16
4		Butane, 2-methoxy-	88	C5H12O	006795-87-5	9
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	9



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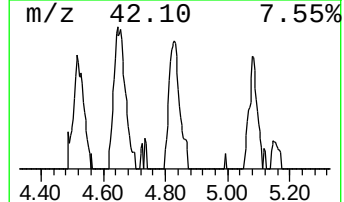
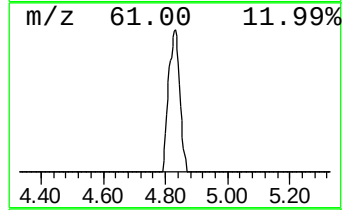
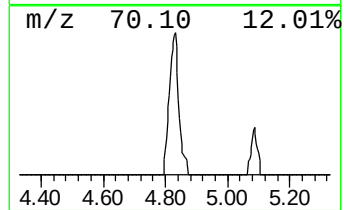
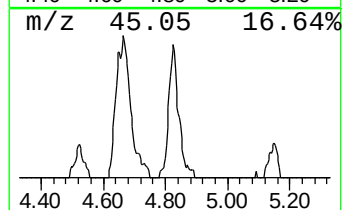
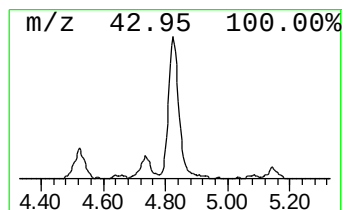
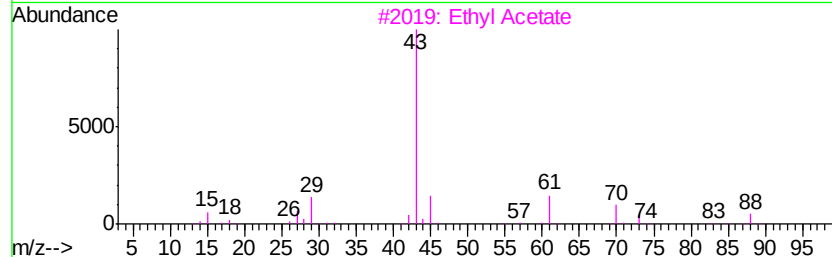
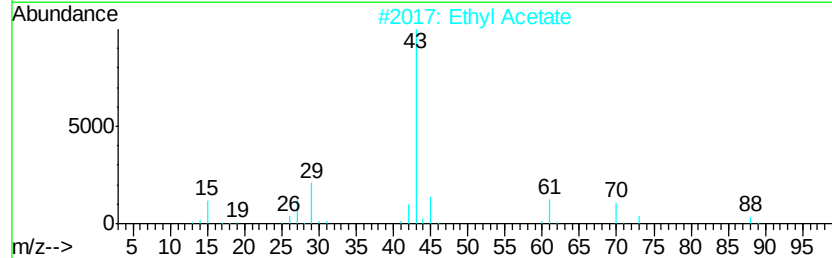
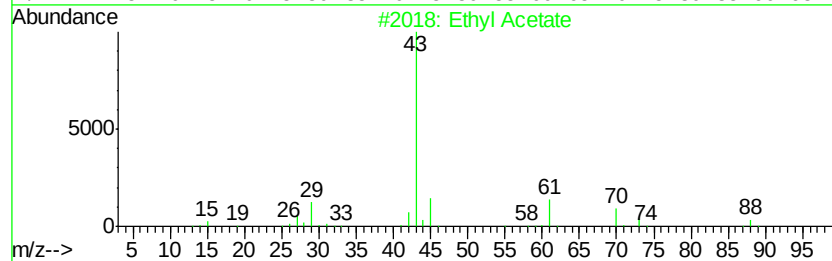
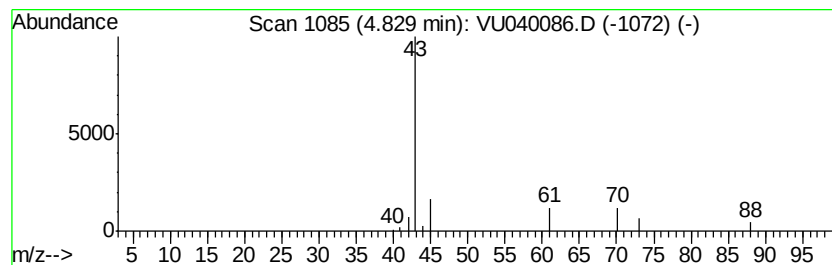
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Ethyl Acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.72 ug/L	43393	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	83
3		Ethyl Acetate	88	C4H8O2	000141-78-6	83
4		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	45
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



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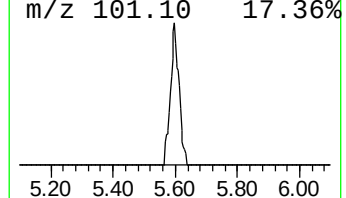
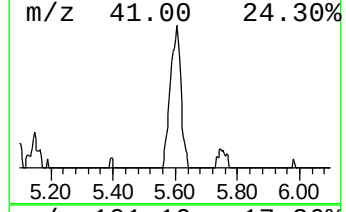
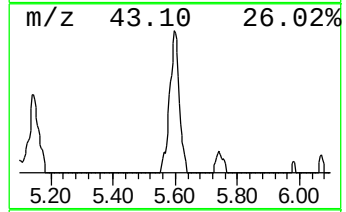
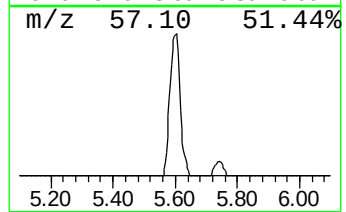
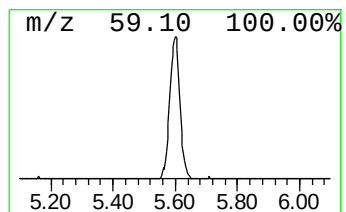
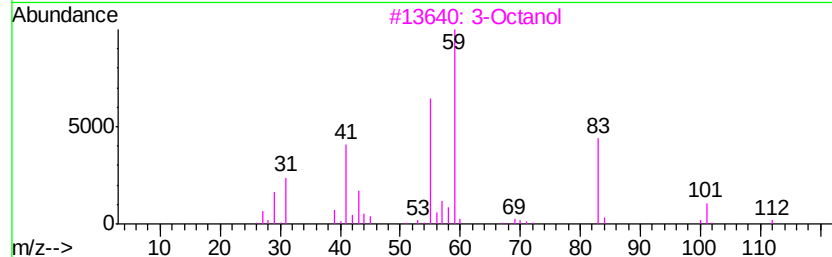
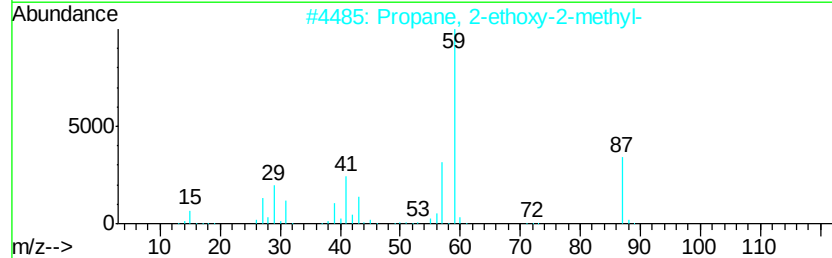
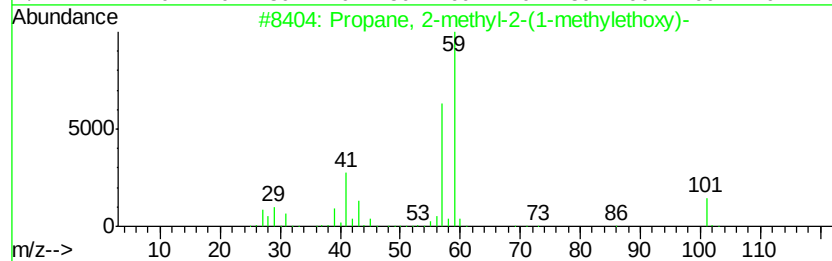
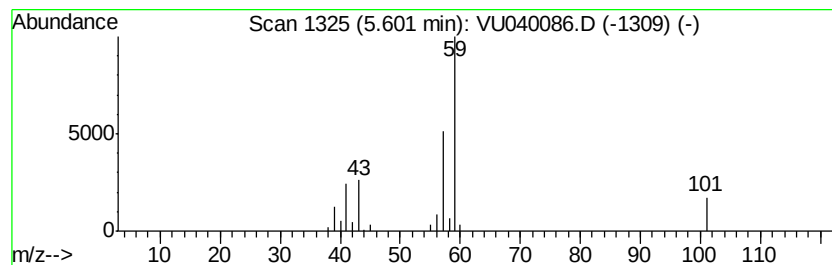
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 Quant Title : TRACE VOA SOM01.0

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

 Peak Number 4 Propane, 2-methyl-2-(1-meth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	0.67 ug/L	40256	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	83
2	Propane, 2-ethoxy-2-methyl-	102	C6H14O		000637-92-3	50
3	3-Octanol	130	C8H18O		000589-98-0	40
4	3-Octanol	130	C8H18O		000589-98-0	40
5	3-Pentanol	88	C5H12O		000584-02-1	39



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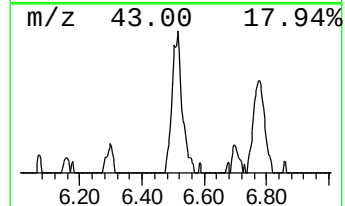
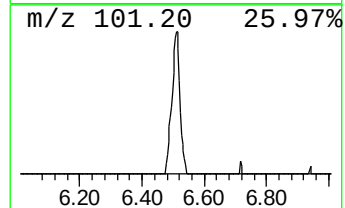
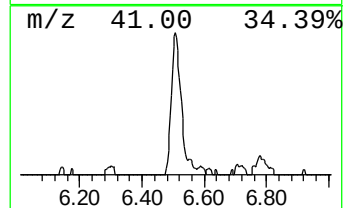
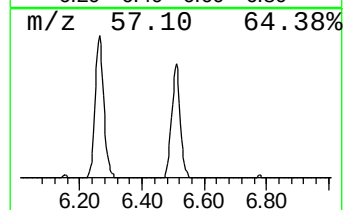
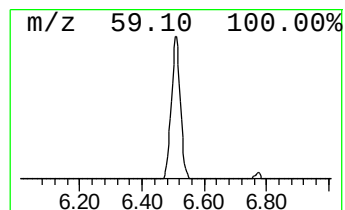
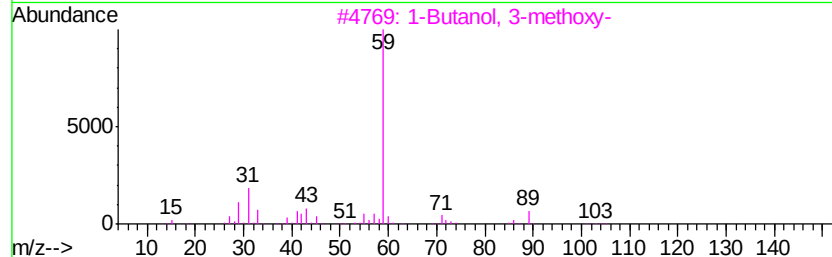
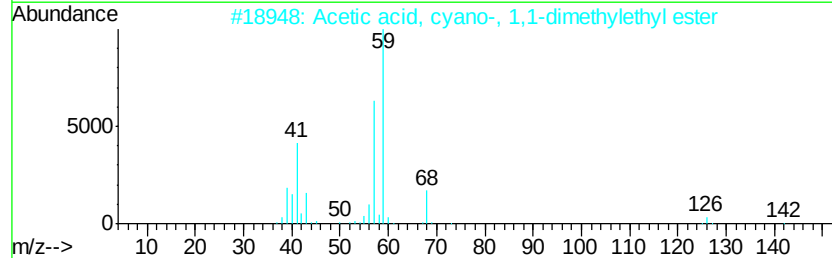
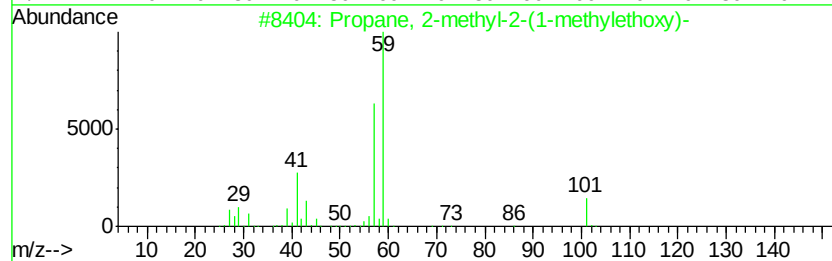
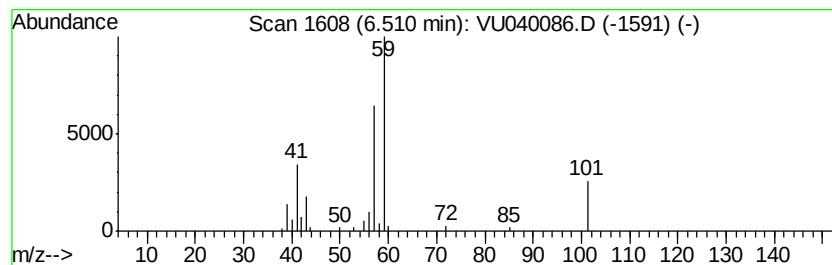
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Quant Title : TRACE VOA SOM01.0

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	0.88 ug/L	52906	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	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	50
3	1-Butanol, 3-methoxy-	104	C5H12O2		002517-43-3	42
4	1-Butanol, 3-methoxy-	104	C5H12O2		002517-43-3	36
5	2-Propanol, 2-methyl-	74	C4H10O		000075-65-0	36



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040086.D
Acq On : 10 Sep 2020 17:14
Operator : SY/MD
Sample : L3961-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y27

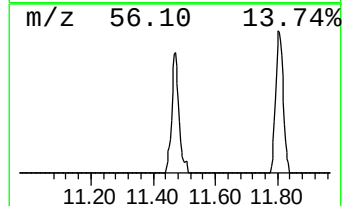
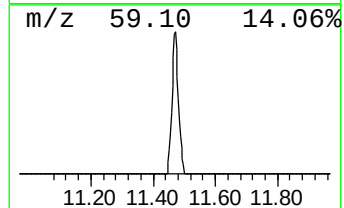
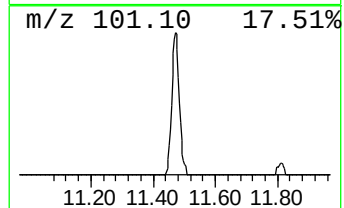
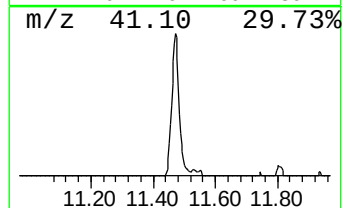
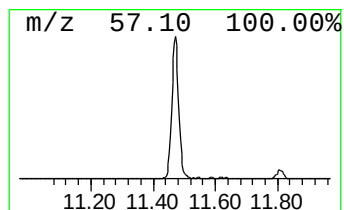
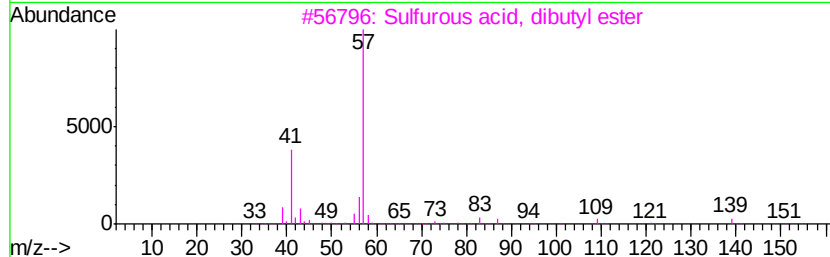
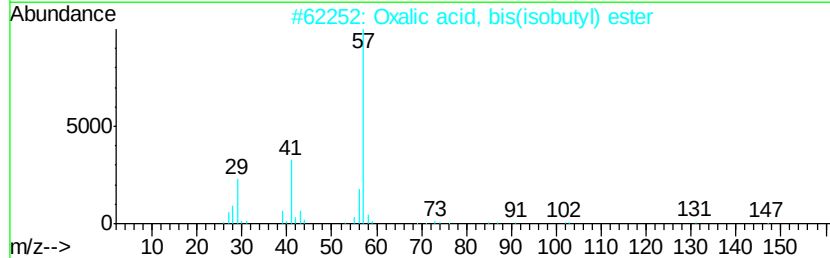
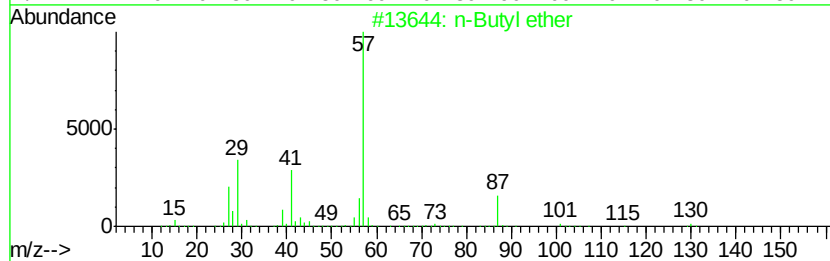
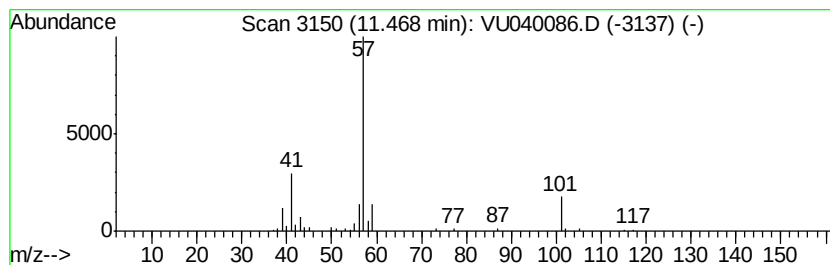
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.72 ug/L	52368	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Butyl ether	130	C8H18O	000142-96-1	47
2		Oxalic acid, bis(isobutyl) ester	202	C10H18O4	1000309-36-8	47
3		Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	43
4		Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	43
5		di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040086.D
Acq On : 10 Sep 2020 17:14
Operator : SY/MD
Sample : L3961-03
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 20 Sample Multiplier: 1

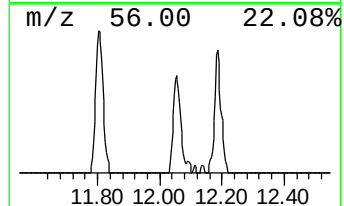
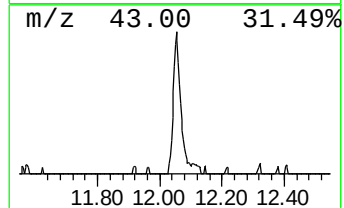
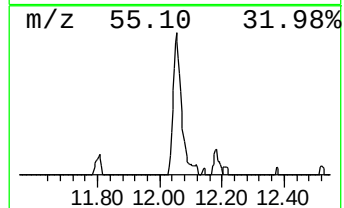
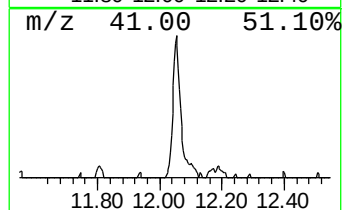
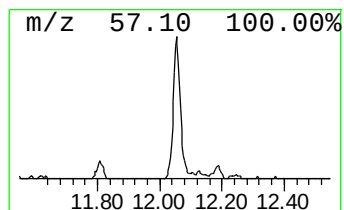
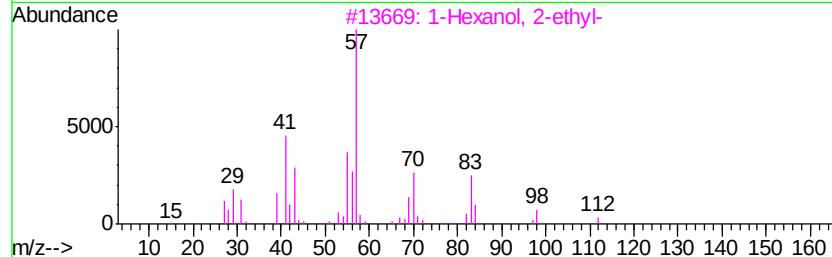
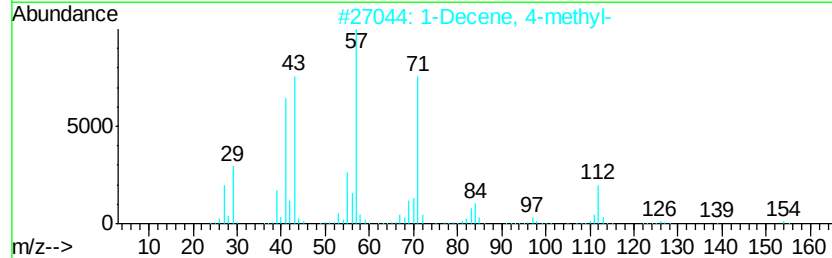
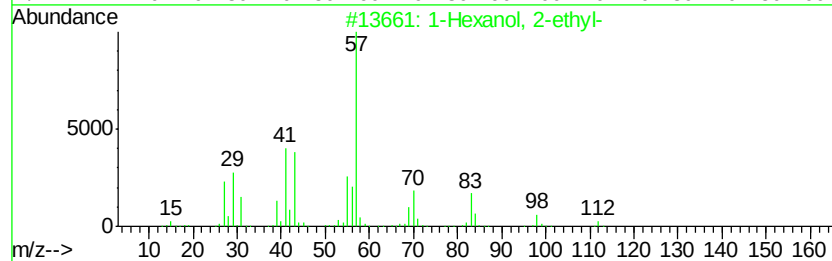
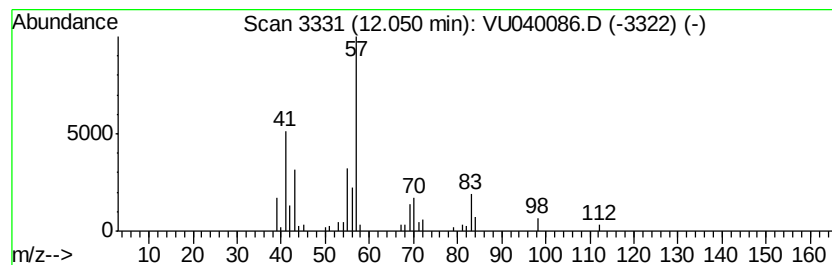
Instrument :
MSVOA_U
ClientSampleId :
F4Y27

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 8 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	0.62 ug/L	45499	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-Decene, 4-methyl-	154 C11H22	013151-29-6	64
3	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	59
4	Octane, 2,3-dimethyl-	142 C10H22	007146-60-3	59
5	2-Heptenal, (Z)-	112 C7H12O	057266-86-1	58



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091020\
Data File : VU040086.D
Acq On : 10 Sep 2020 17:14
Operator : SY/MD
Sample : L3961-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y27

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	7.2	ug/L	435603	1	6.26	301526	5.0
Propane, 2-ethoxy...	4.52	1.6	ug/L	97446	1	6.26	301526	5.0
Ethyl Acetate	4.83	0.7	ug/L	43393	1	6.26	301526	5.0
Propane, 2-methyl...	5.60	0.7	ug/L	40256	1	6.26	301526	5.0
Acetic acid, cyan...	6.51	0.9	ug/L	52906	1	6.26	301526	5.0
unknown-01	11.47	0.7	ug/L	52368	3	11.81	365761	5.0
1-Hexanol, 2-ethyl-	12.05	0.6	ug/L	45499	3	11.81	365761	5.0