

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
 Data File : VU040085.D
 Acq On : 10 Sep 2020 16:51
 Operator : SY/MD
 Sample : L3961-02
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4Y26

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	1.494	43	48	57	rVB	9461	9192	2.03%	0.208%
2	1.604	71	82	92	rVB	55155	68004	15.05%	1.540%
3	1.922	170	181	190	rBV	41219	52899	11.71%	1.198%
4	2.080	215	230	231	rBV	5119	9877	2.19%	0.224%
5	2.581	374	386	397	rBV	86930	141313	31.27%	3.201%
6	2.652	397	408	428	rVB2	26783	63450	14.04%	1.437%
7	2.826	441	462	513	rBV2	68148	377713	83.58%	8.555%
8	3.382	618	635	653	rVB2	26728	62053	13.73%	1.405%
9	3.890	781	793	806	rBV2	3635	7412	1.64%	0.168%
10	4.018	818	833	848	rBV4	3831	9962	2.20%	0.226%
11	4.520	973	989	1008	rBV2	35897	90827	20.10%	2.057%
12	4.649	1013	1029	1050	rBV	68904	178386	39.48%	4.040%
13	4.825	1072	1084	1098	rVB3	15987	35555	7.87%	0.805%
14	5.083	1149	1164	1180	rBV3	75568	166788	36.91%	3.778%
15	5.597	1311	1324	1340	rBV4	16301	36733	8.13%	0.832%
16	5.742	1346	1369	1388	rBV2	146185	372855	82.51%	8.445%
17	6.263	1517	1531	1552	rBV2	154383	289236	64.01%	6.551%
18	6.507	1595	1607	1626	rBV3	23059	47280	10.46%	1.071%
19	6.703	1655	1668	1683	rBV3	90324	177325	39.24%	4.016%
20	6.780	1683	1692	1704	rVB8	3408	7181	1.59%	0.163%
21	7.166	1800	1812	1823	rBV4	8264	15112	3.34%	0.342%
22	7.227	1823	1831	1841	rVB7	5447	10792	2.39%	0.244%
23	7.304	1841	1855	1866	rBV4	13242	23983	5.31%	0.543%
24	7.575	1927	1939	1952	rBV	47650	81076	17.94%	1.836%
25	7.726	1969	1986	1996	rBV5	7848	15513	3.43%	0.351%
26	7.906	2017	2042	2058	rBV	169896	320244	70.87%	7.254%
27	8.185	2116	2129	2142	rBV3	29898	50084	11.08%	1.134%
28	8.510	2218	2230	2240	rVB4	5943	10613	2.35%	0.240%
29	8.639	2256	2270	2299	rBV	249649	451893	100.00%	10.235%
30	8.931	2348	2361	2378	rVB2	7071	14777	3.27%	0.335%
31	9.420	2499	2513	2528	rBV	226900	376184	83.25%	8.521%
32	9.761	2606	2619	2628	rBV7	2475	6167	1.36%	0.140%
33	10.755	2916	2928	2945	rVB2	71099	117626	26.03%	2.664%
34	11.472	3139	3151	3164	rBV2	31465	51793	11.46%	1.173%

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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

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Title : TRACE VOA SOM01.0

35	11.806	3243	3255	3273	rVB	217434	348716	77.17%	7.898%
36	12.053	3322	3332	3350	rBV3	23515	40065	8.87%	0.907%
37	12.189	3361	3374	3388	rVB	172074	276335	61.15%	6.259%

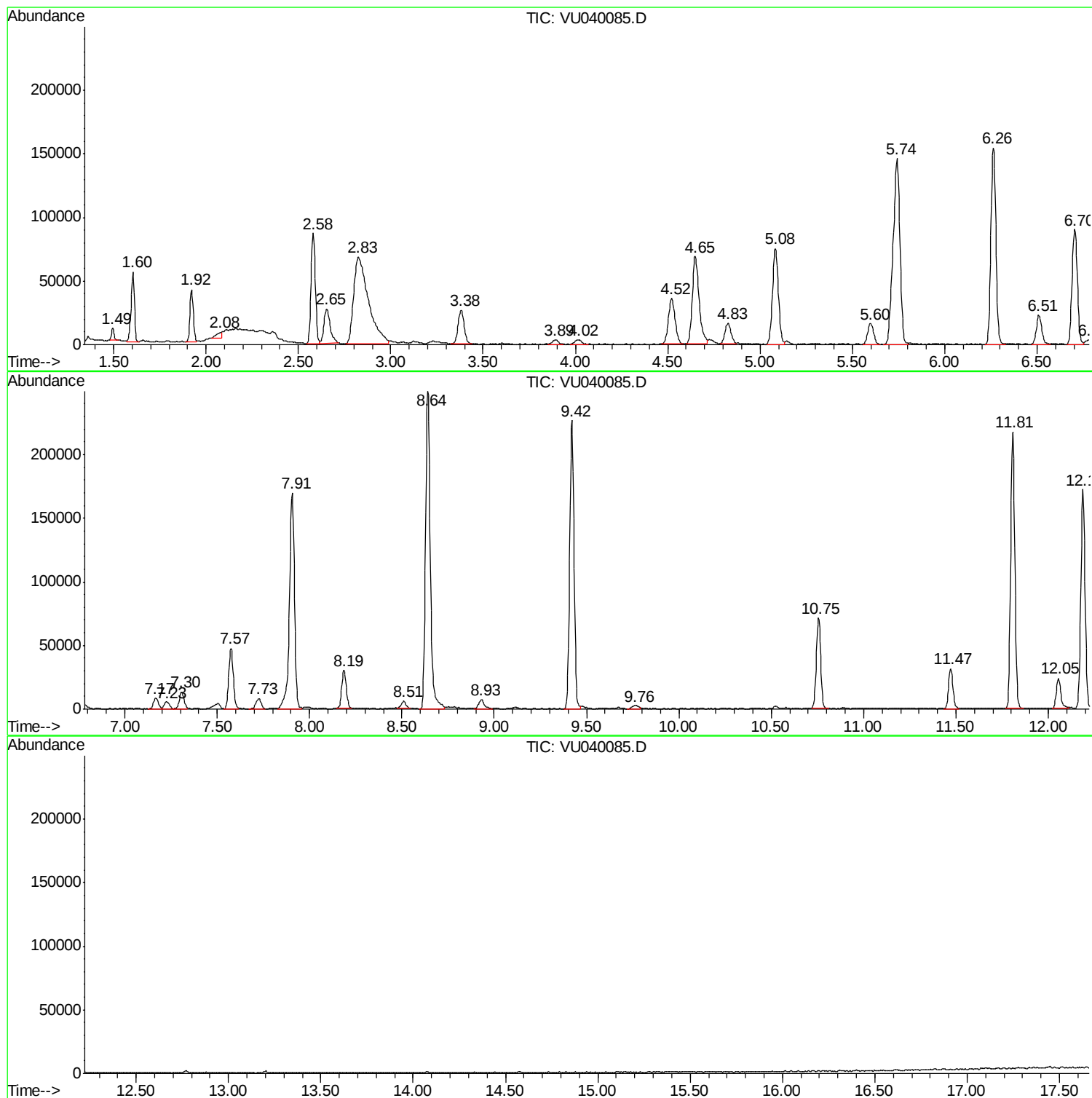
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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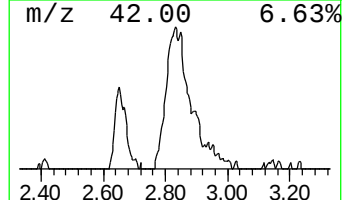
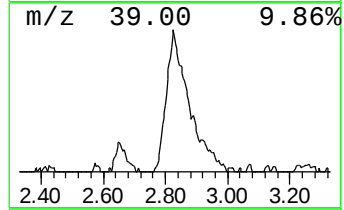
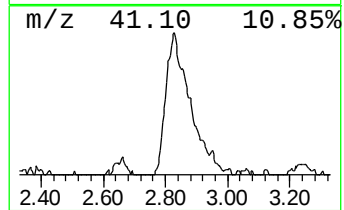
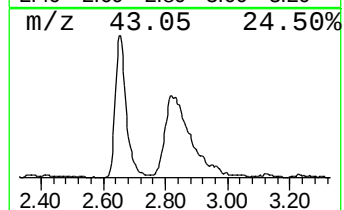
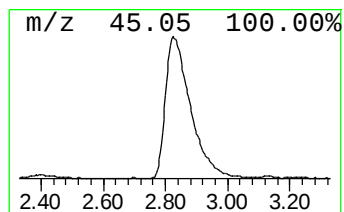
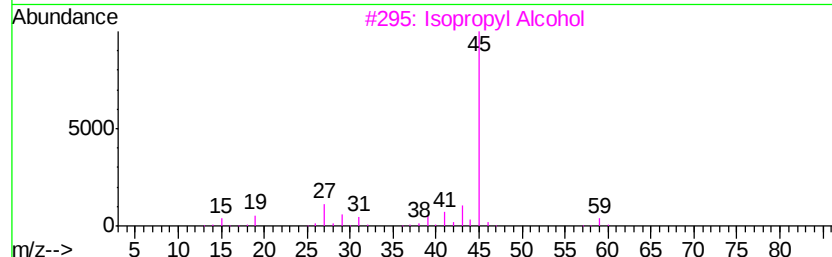
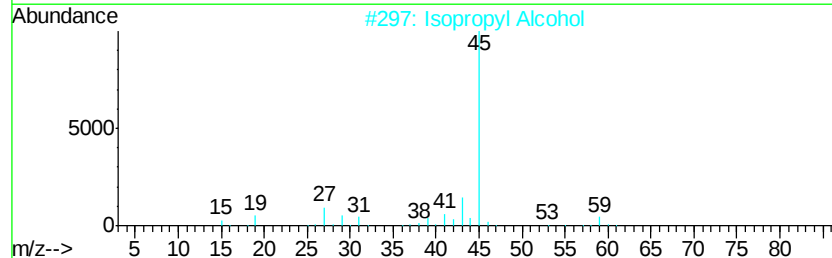
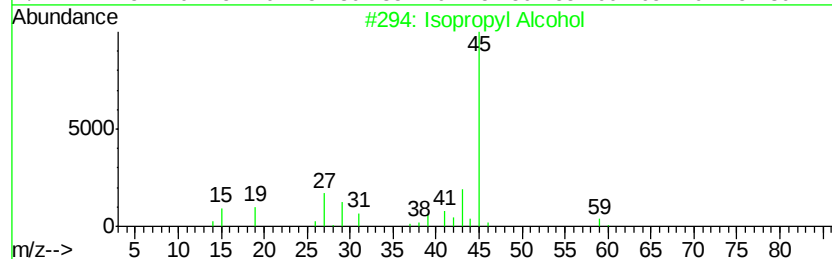
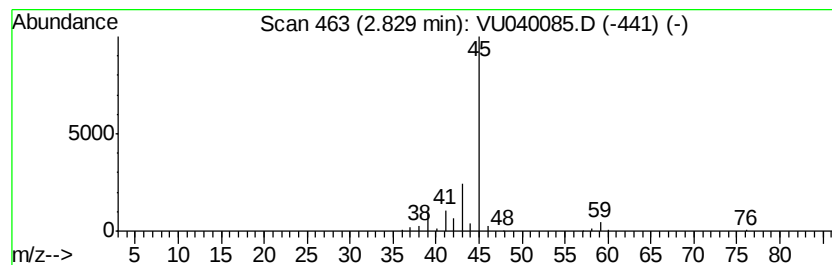
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Quant Title : TRACE VOA SOM01.0

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	6.53 ug/L	377713	1,4-Difluorobenzene	6.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
5			Hydrazine, ethyl-	60	C2H8N2	000624-80-6	40



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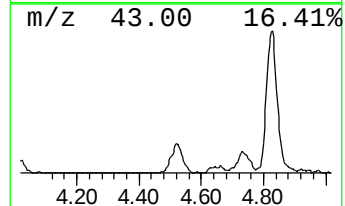
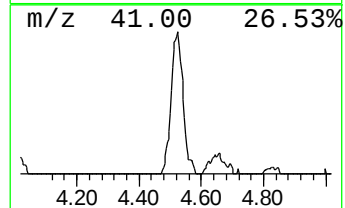
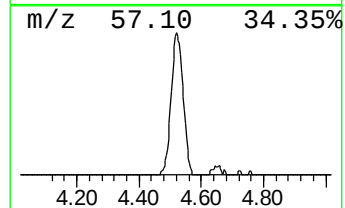
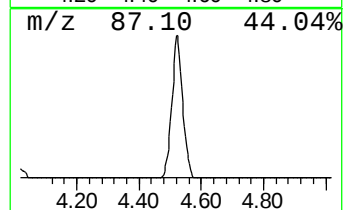
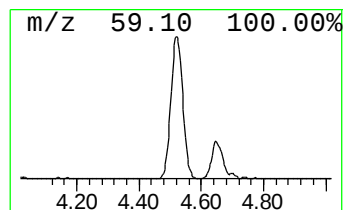
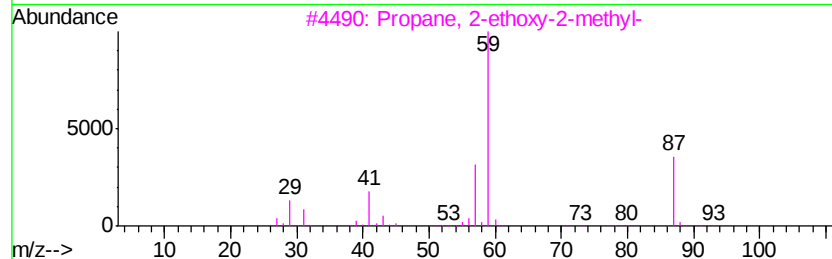
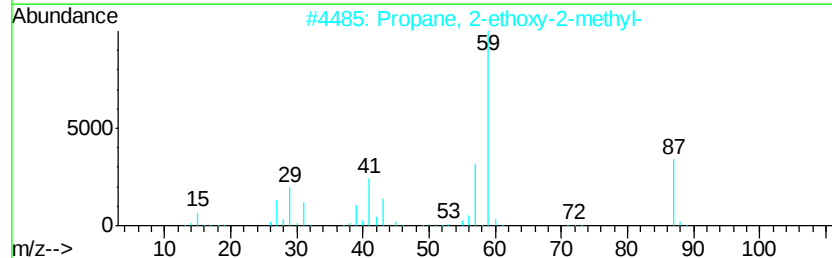
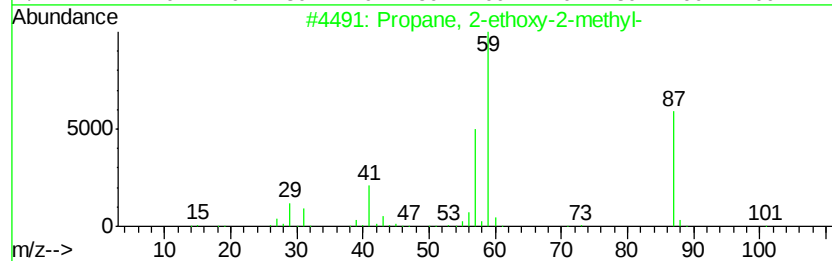
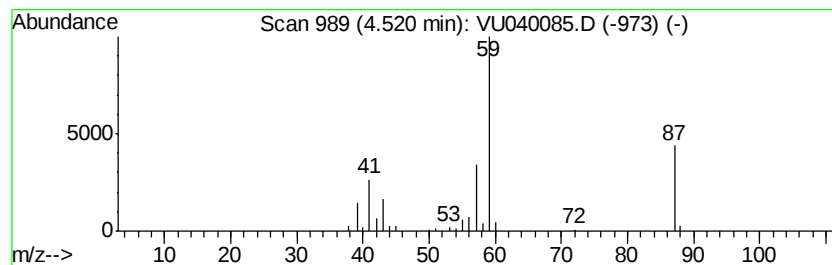
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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	1.57 ug/L	90827	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	43
5		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40



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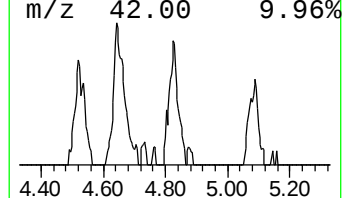
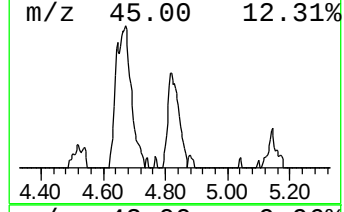
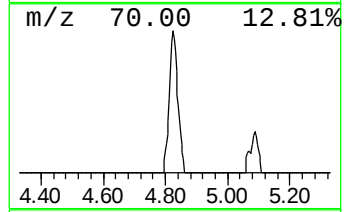
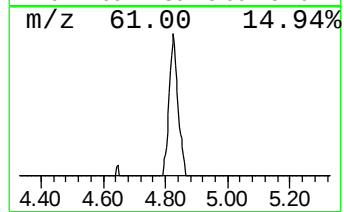
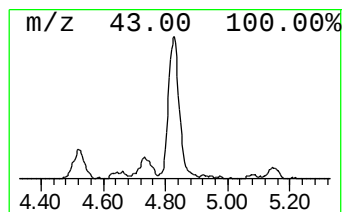
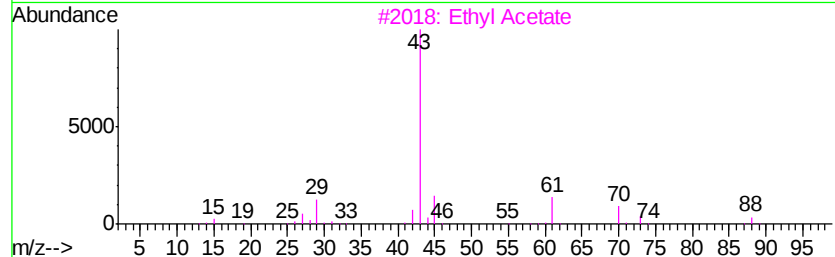
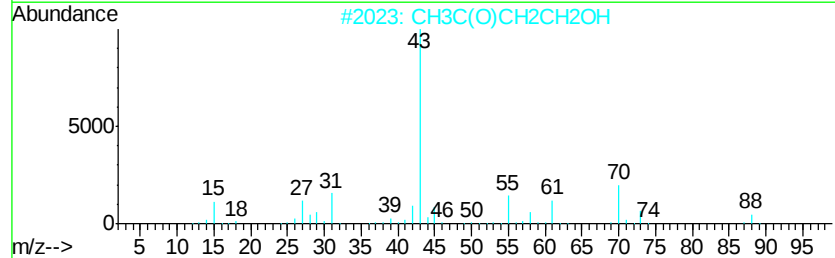
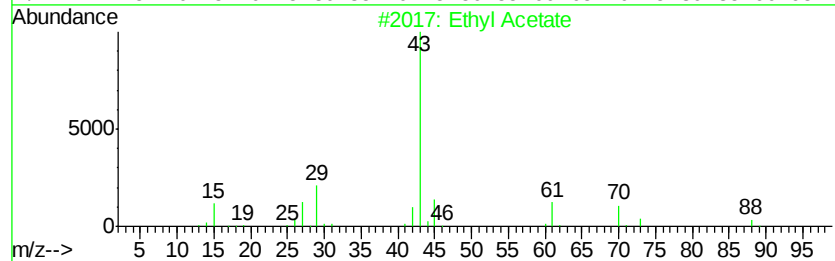
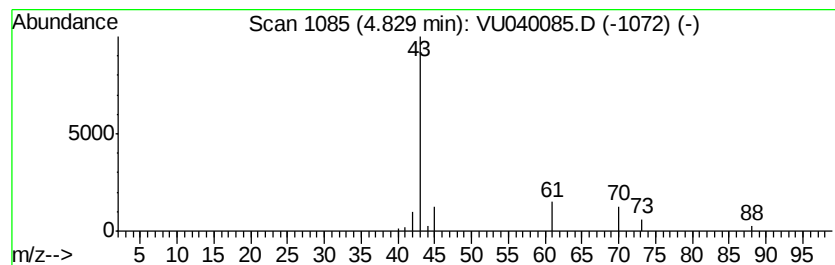
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethyl Acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	0.61 ug/L	35555	1,4-Difluorobenzene	6.26

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



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Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

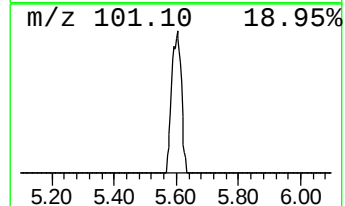
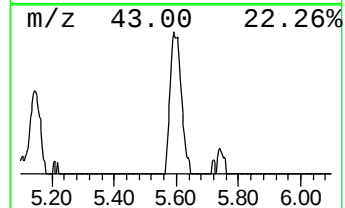
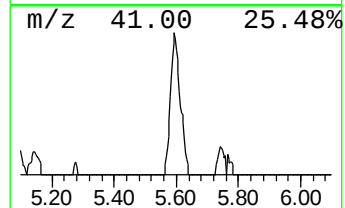
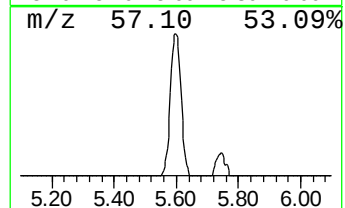
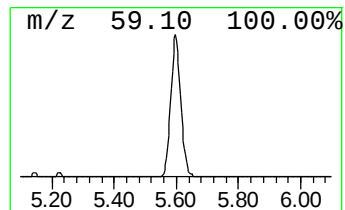
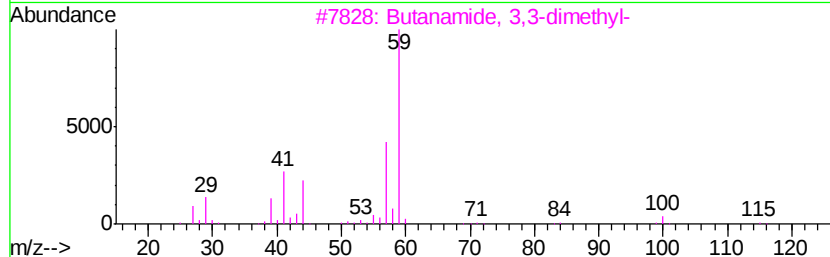
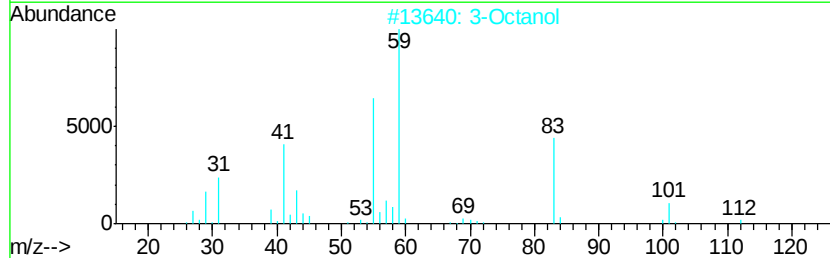
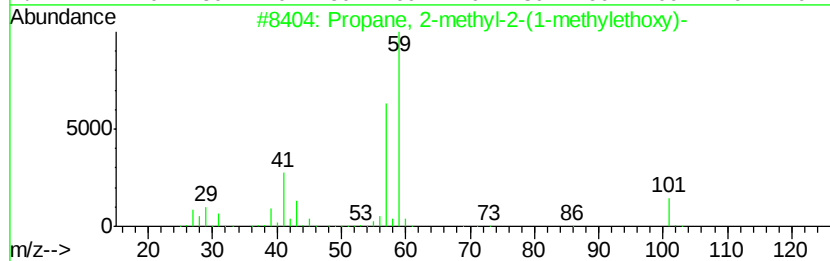
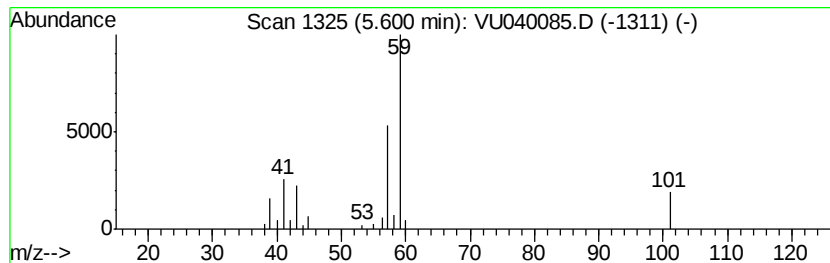
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.60	0.64 ug/L	36733	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	3-Octanol	130	C8H18O	000589-98-0	74
3	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	56
4	2-Hexanone, 3-hydroxy-3,5-dimethyl-	144	C8H16O2	006321-14-8	43
5	3-Octanol	130	C8H18O	000589-98-0	40



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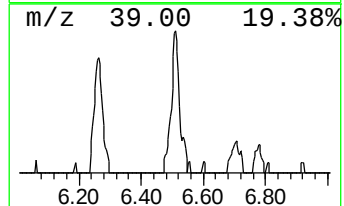
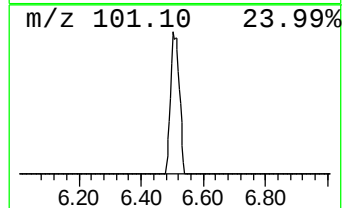
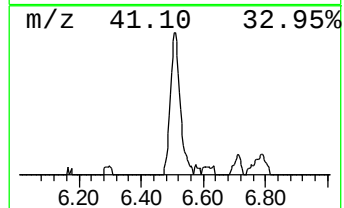
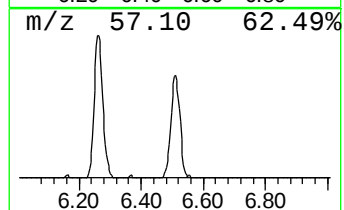
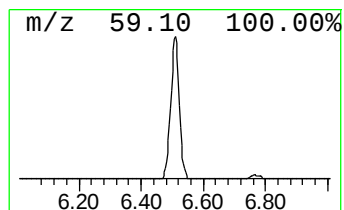
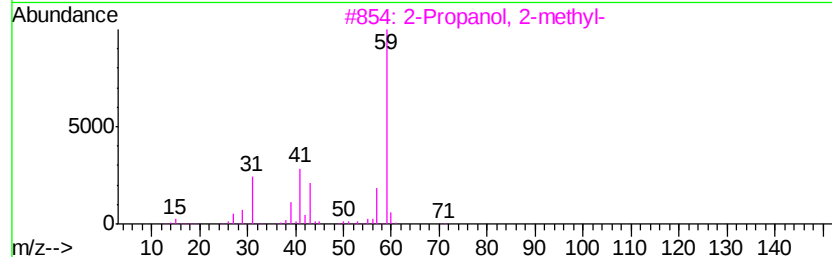
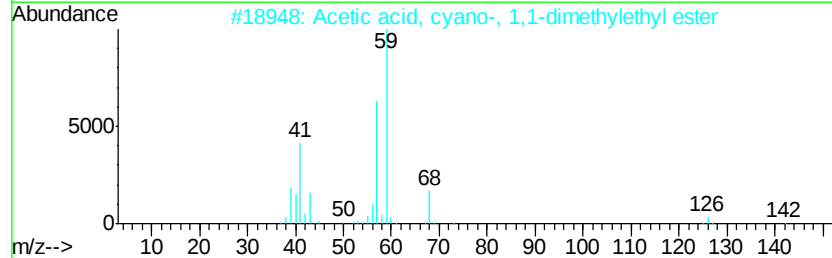
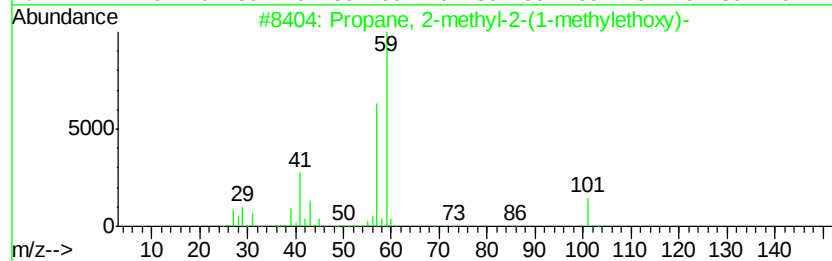
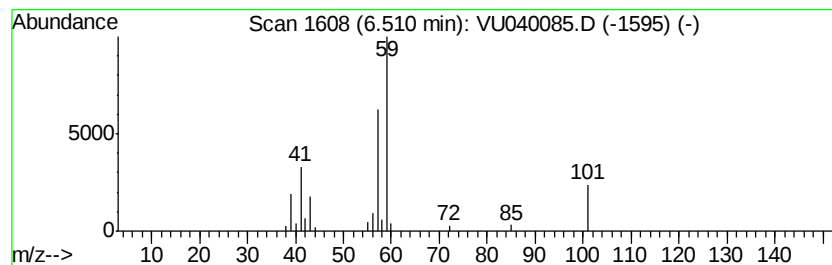
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	0.82 ug/L	47280	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	72	
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	64	
3	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	53	
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	45	
5	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	40	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040085.D
Acq On : 10 Sep 2020 16:51
Operator : SY/MD
Sample : L3961-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y26

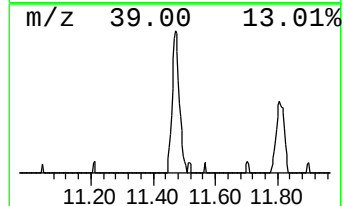
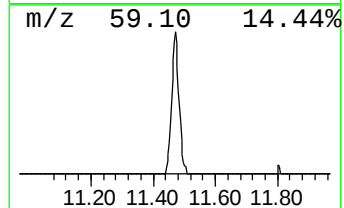
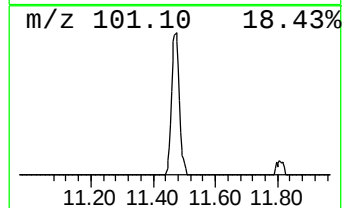
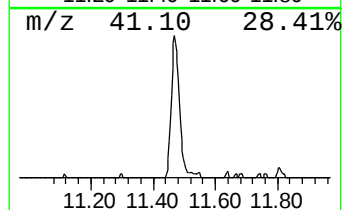
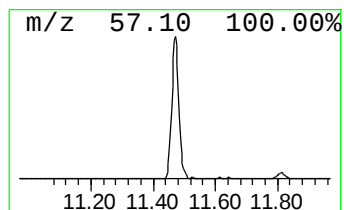
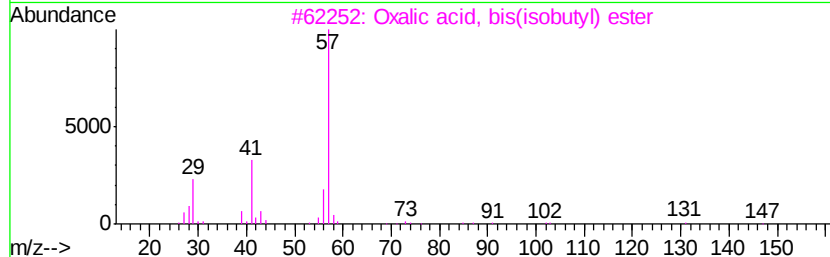
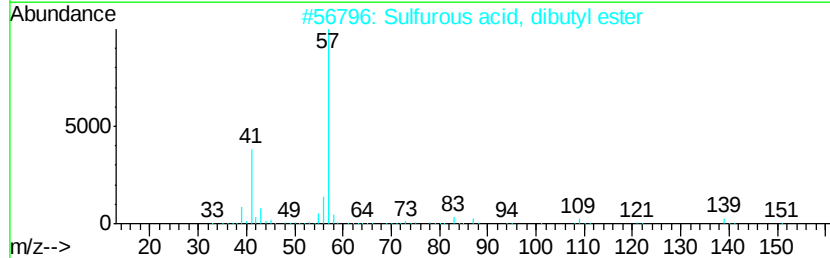
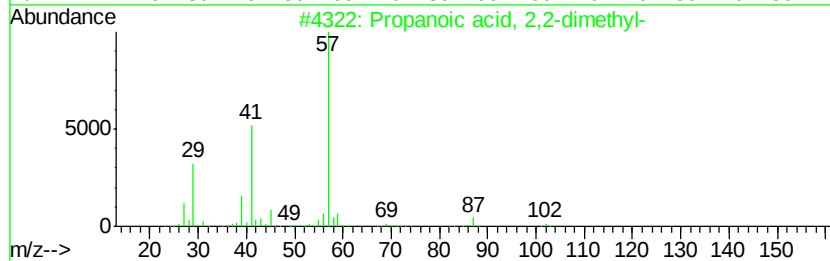
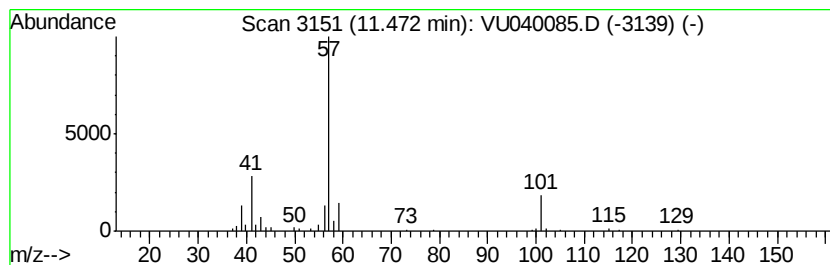
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Propanoic acid, 2,2-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	0.74 ug/L	51793	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	53
2		Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	47
3		Oxalic acid, bis(isobutyl) ester	202	C10H18O4	1000309-36-8	47
4		di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	42
5		Propanedioic acid, oxo-, bis(2-m...	230	C11H18O5	092778-43-3	38



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040085.D
Acq On : 10 Sep 2020 16:51
Operator : SY/MD
Sample : L3961-02
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y26

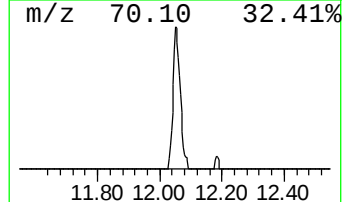
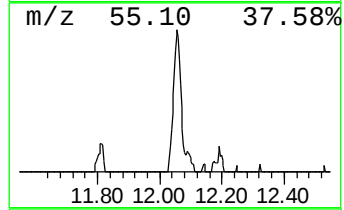
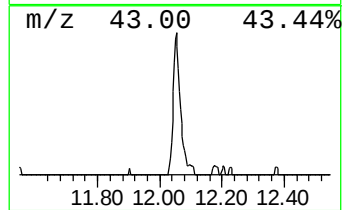
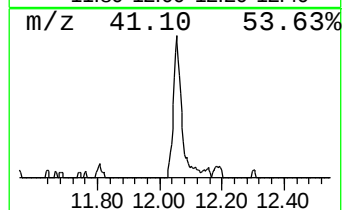
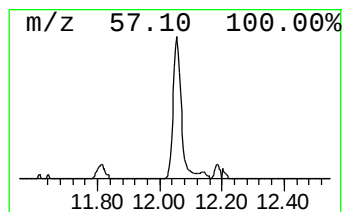
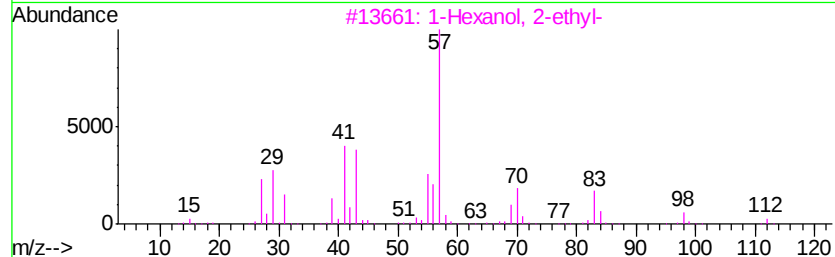
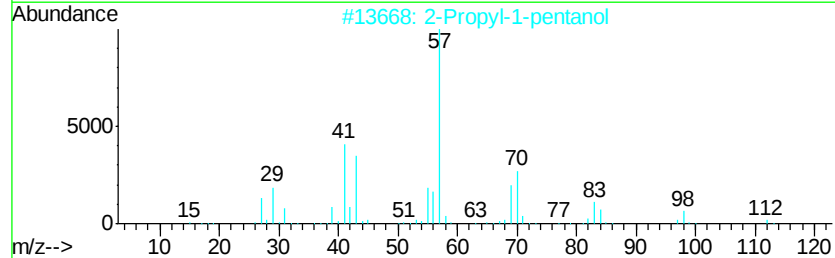
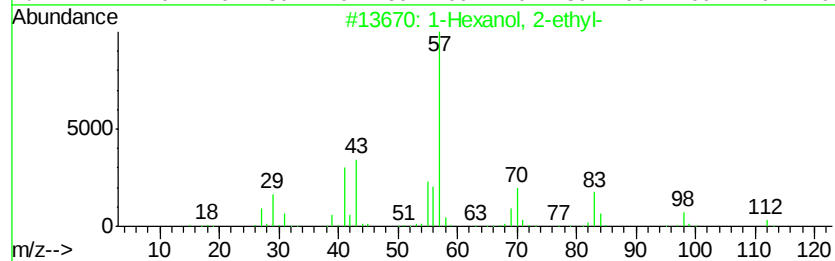
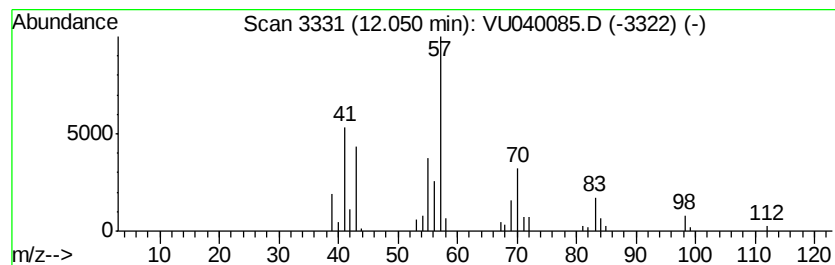
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	0.57 ug/L	40065	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	64



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091020\
Data File : VU040085.D
Acq On : 10 Sep 2020 16:51
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Sample : L3961-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y26

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	6.5	ug/L	377713	1	6.26	289236	5.0
Propane, 2-ethoxy...	4.52	1.6	ug/L	90827	1	6.26	289236	5.0
Ethyl Acetate	4.83	0.6	ug/L	35555	1	6.26	289236	5.0
Propane, 2-methyl...	5.60	0.6	ug/L	36733	1	6.26	289236	5.0
Acetic acid, cyan...	6.51	0.8	ug/L	47280	1	6.26	289236	5.0
Propanoic acid, 2...	11.47	0.7	ug/L	51793	3	11.81	348716	5.0
1-Hexanol, 2-ethyl-	12.05	0.6	ug/L	40065	3	11.81	348716	5.0