

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU082120\
 Data File : VU039932.D
 Acq On : 21 Aug 2020 16:50
 Operator : SY/MD
 Sample : L3776-08
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4Y07

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\SOMUTR081920WMA.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	1.363	3	7	21	rVB2	21430	21865	5.27%	0.545%
2	1.604	72	82	93	rBV	49057	63597	15.33%	1.585%
3	1.922	171	181	191	rBV	42637	56150	13.54%	1.399%
4	2.578	375	385	398	rVB	63029	101505	24.47%	2.530%
5	2.655	398	409	425	rBV2	17649	40413	9.74%	1.007%
6	2.848	441	469	519	rBV2	45207	321597	77.53%	8.015%
7	3.382	623	635	650	rVB3	9530	20726	5.00%	0.517%
8	3.890	772	793	818	rBV	123323	294946	71.11%	7.350%
9	4.006	818	829	832	rBV5	2886	4228	1.02%	0.105%
10	4.527	973	991	1009	rVB3	47382	120292	29.00%	2.998%
11	4.652	1014	1030	1052	rBV2	62420	172970	41.70%	4.311%
12	4.829	1070	1085	1107	rVB	19286	44790	10.80%	1.116%
13	5.083	1148	1164	1178	rBV	68702	153570	37.02%	3.827%
14	5.597	1307	1324	1343	rBV4	23168	54589	13.16%	1.360%
15	5.742	1349	1369	1385	rBV3	134380	348355	83.99%	8.681%
16	6.263	1517	1531	1554	rBV	98717	190367	45.90%	4.744%
17	6.510	1595	1608	1625	rBV	38153	75854	18.29%	1.890%
18	6.703	1654	1668	1686	rBV2	86446	166349	40.11%	4.146%
19	7.166	1802	1812	1822	rBV6	2647	4201	1.01%	0.105%
20	7.311	1847	1857	1864	rBV7	2802	4599	1.11%	0.115%
21	7.469	1898	1906	1922	rBV4	5359	10950	2.64%	0.273%
22	7.575	1928	1939	1955	rBV	42577	73592	17.74%	1.834%
23	7.726	1975	1986	1993	rVB9	2832	6329	1.53%	0.158%
24	7.906	2018	2042	2058	rBV	153246	263684	63.57%	6.571%
25	7.973	2058	2063	2075	rVB4	2836	4696	1.13%	0.117%
26	8.186	2117	2129	2141	rBV2	29581	52151	12.57%	1.300%
27	8.639	2257	2270	2296	rBV	240962	414779	100.00%	10.337%
28	8.928	2353	2360	2368	rBV5	2412	4548	1.10%	0.113%
29	9.420	2498	2513	2531	rBV	155295	251960	60.75%	6.279%
30	10.755	2912	2928	2943	rBV2	64853	107890	26.01%	2.689%
31	11.472	3141	3151	3166	rBV	34510	51677	12.46%	1.288%
32	11.809	3245	3256	3267	rVB	147950	229202	55.26%	5.712%
33	12.054	3322	3332	3344	rBV2	16075	26312	6.34%	0.656%
34	12.189	3359	3374	3387	rBV	157896	253917	61.22%	6.328%

LSC Area Percent Report

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y07

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\SOMUTR081920WMA.M
Title : TRACE VOA SOM01.0

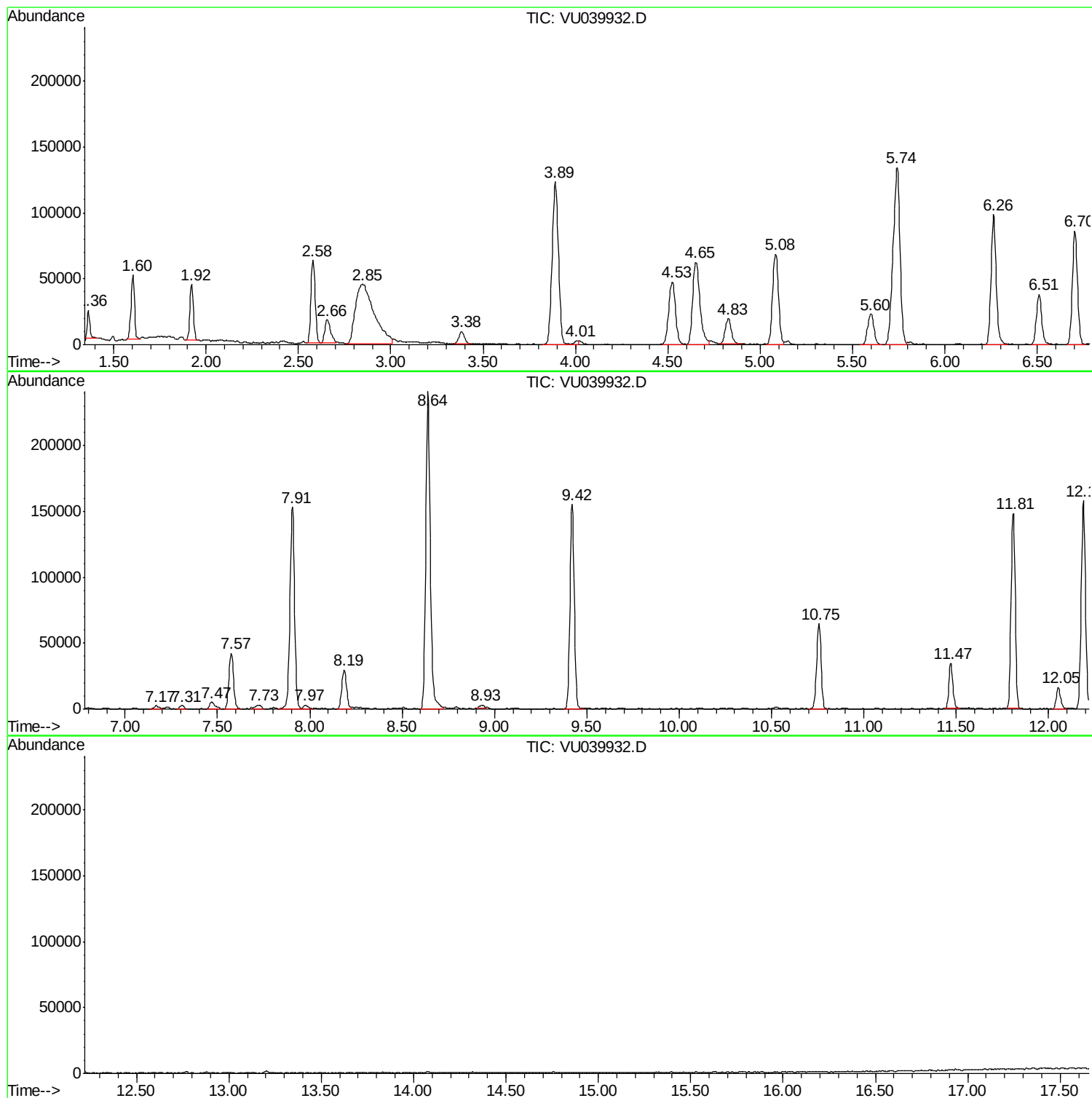
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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



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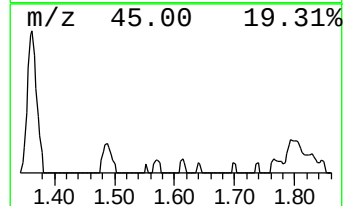
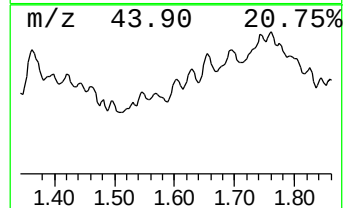
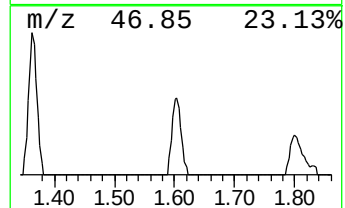
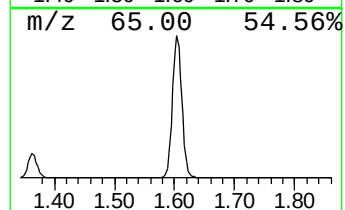
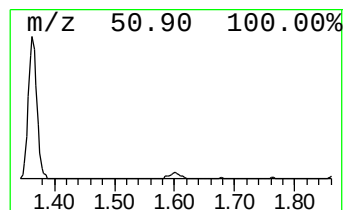
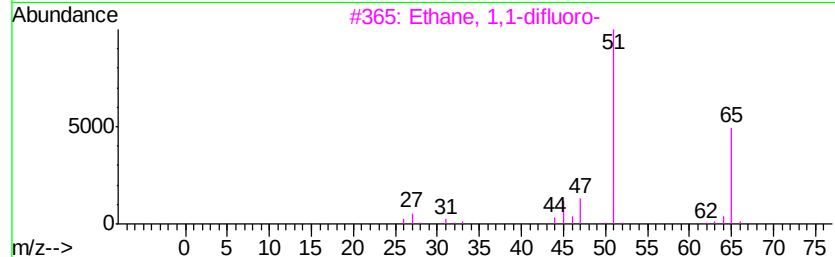
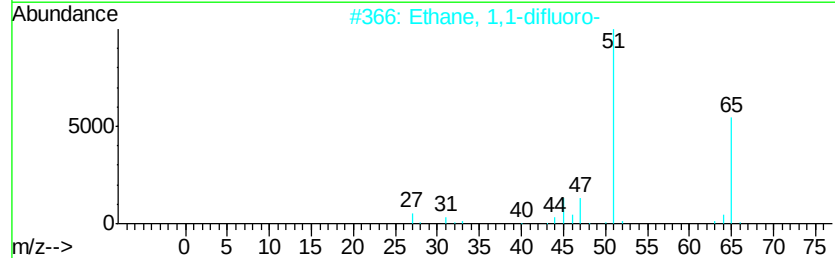
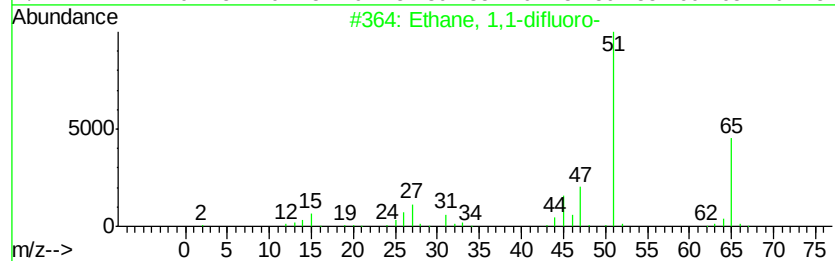
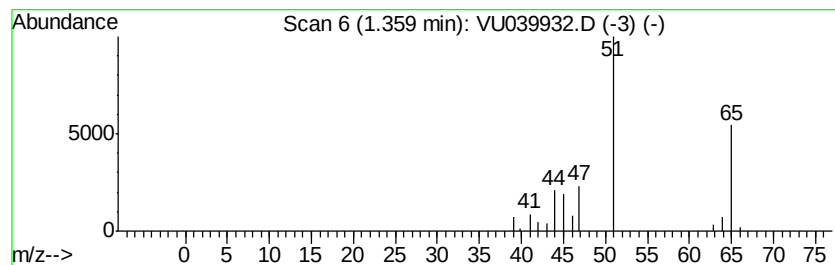
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.36	0.57 ug/L	21865	1,4-Difluorobenzene	6.26

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
2			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
3			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
4			Propiolonitrile	51	C3HN	001070-71-9	3
5			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2



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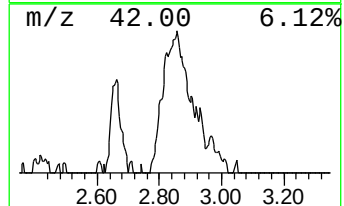
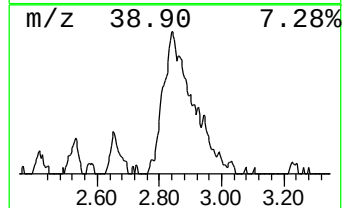
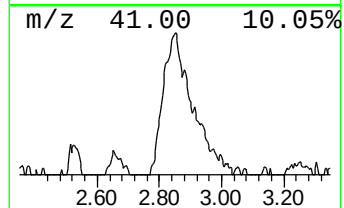
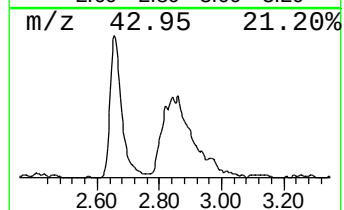
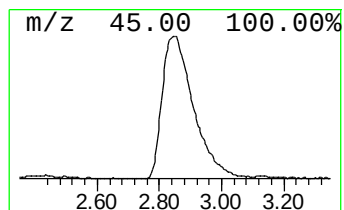
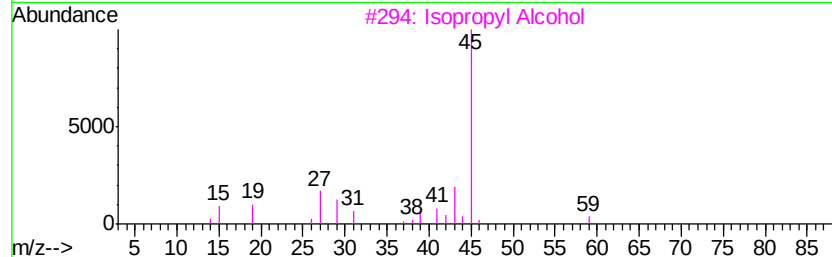
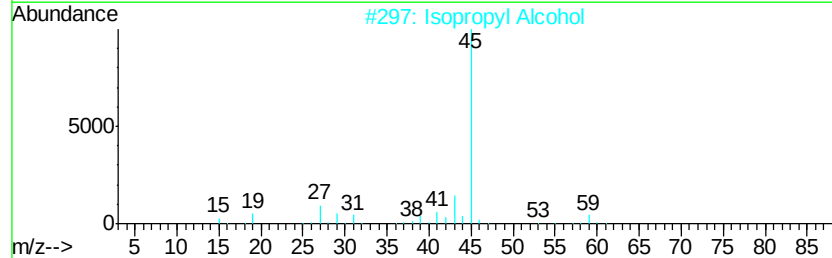
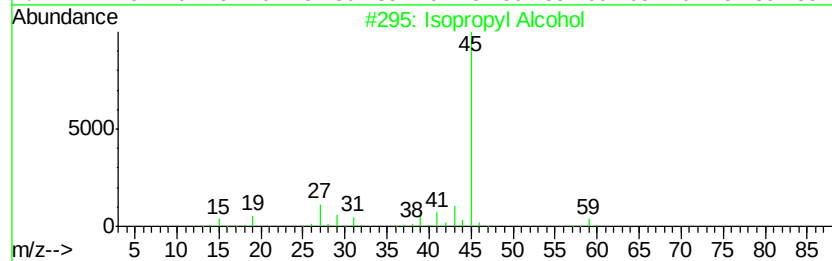
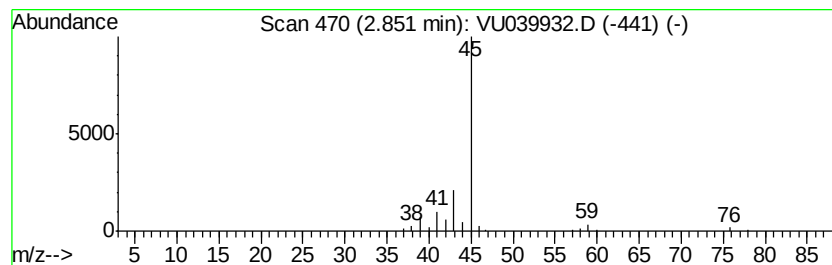
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.85	8.45 ug/L	321597	1,4-Difluorobenzene	6.26	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	Isopropyl Alcohol	60	C3H8O	000067-63-0	72
5	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40



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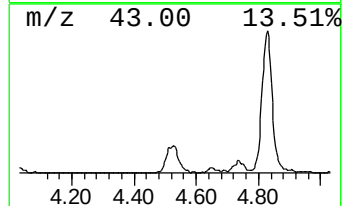
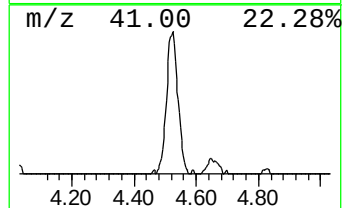
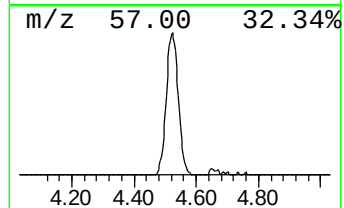
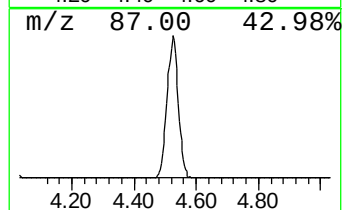
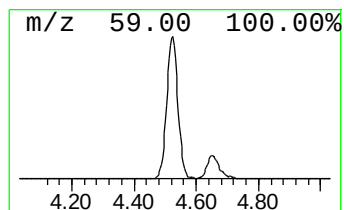
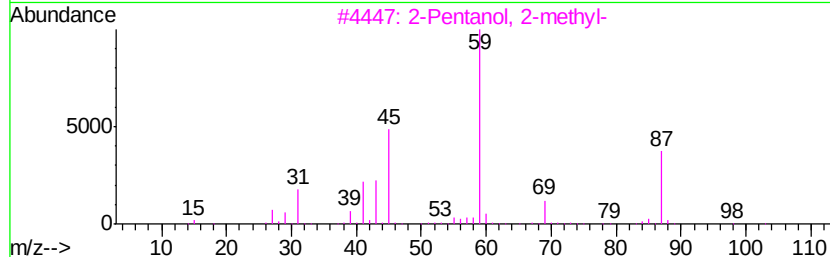
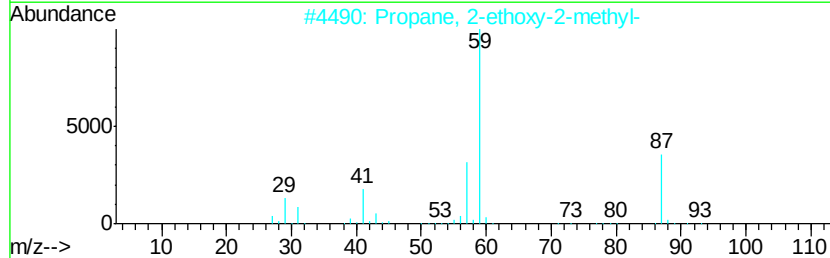
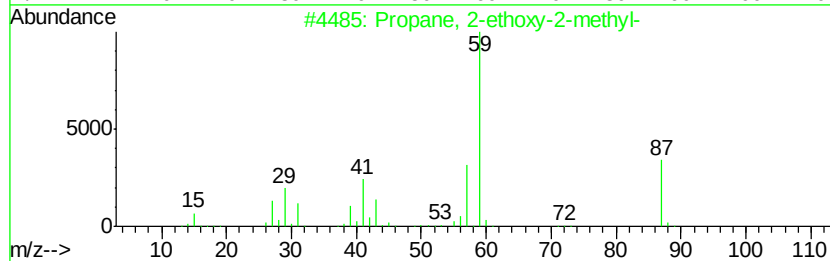
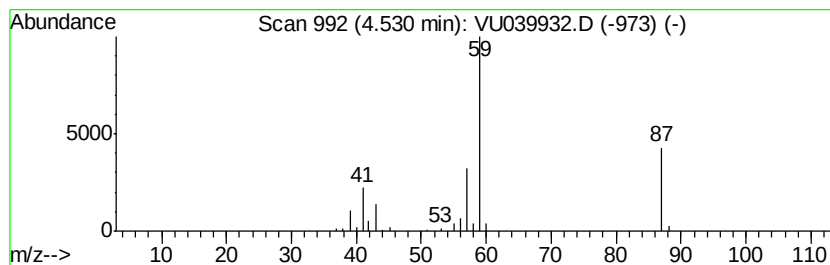
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.53	3.16 ug/L	120292	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	83
3		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
4		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	40
5		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	40



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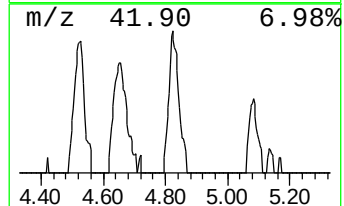
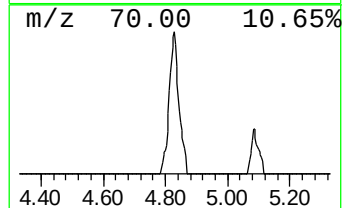
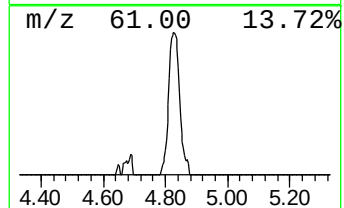
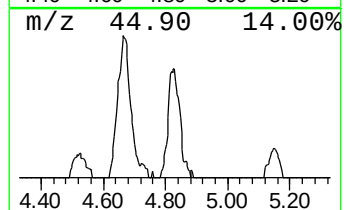
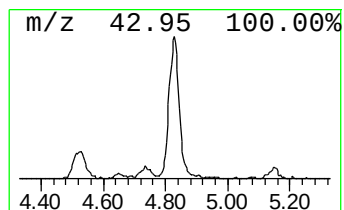
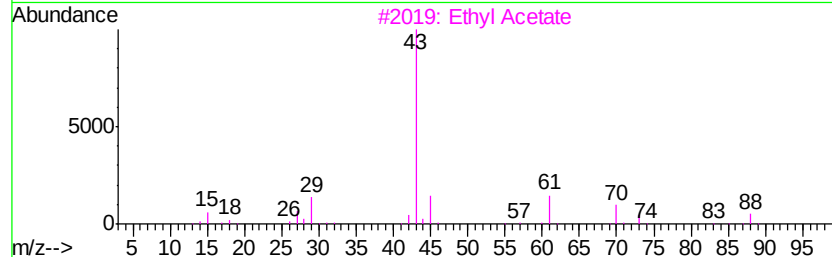
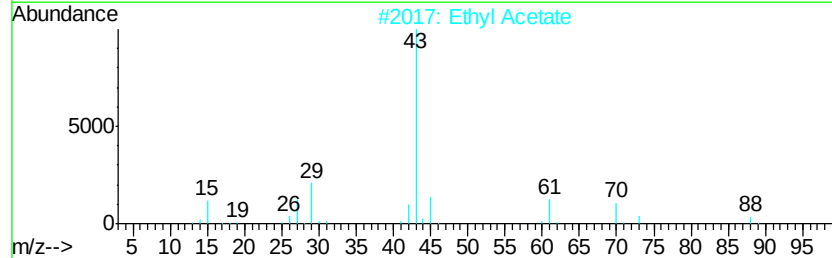
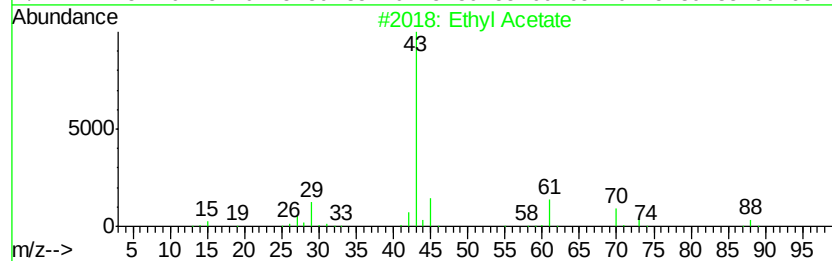
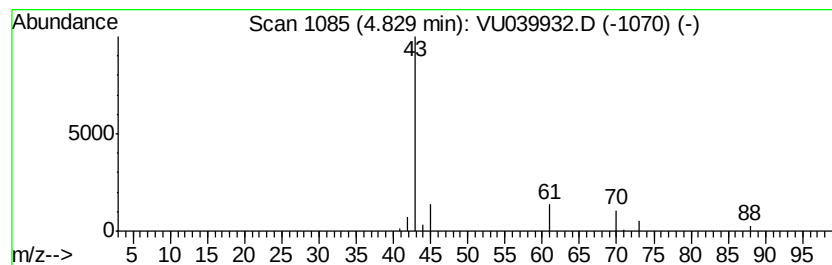
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Ethyl Acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	1.18 ug/L	44790	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	83
4		Ethyl Acetate	88	C4H8O2	000141-78-6	83
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	36



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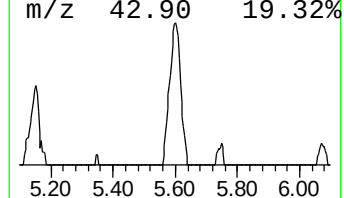
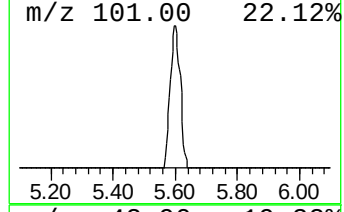
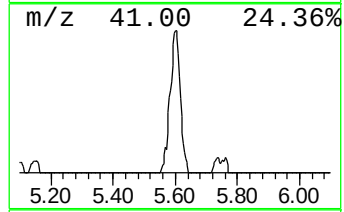
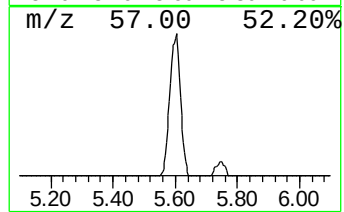
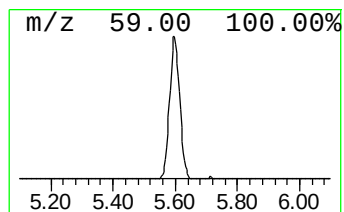
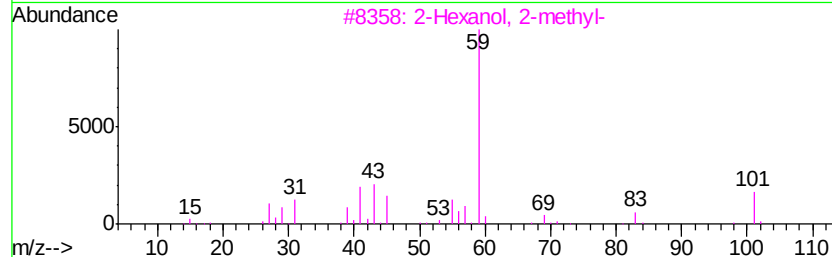
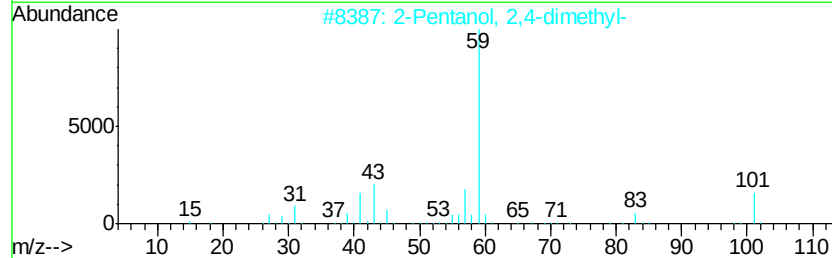
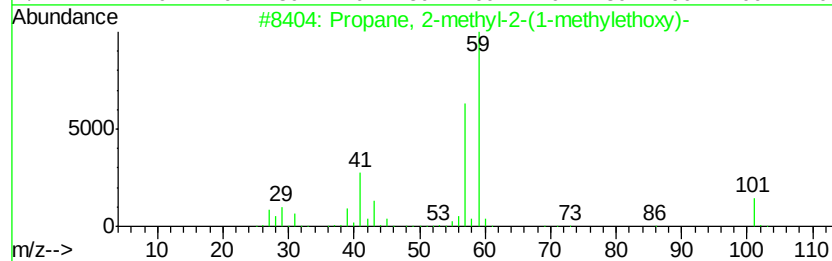
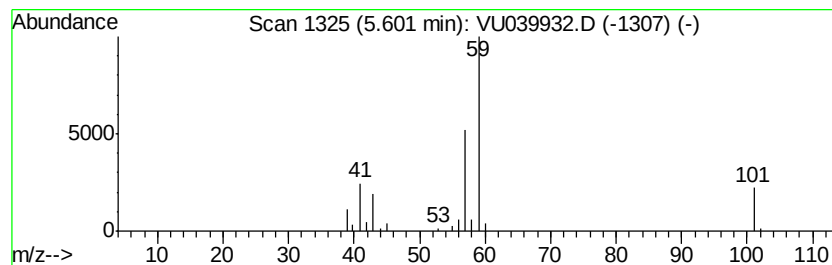
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propane, 2-methyl-2-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	1.43 ug/L	54589	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	78	
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	43	
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	39	
4	3-Hexanol	102	C6H14O	000623-37-0	38	
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	38	



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ClientSampleId :
F4Y07

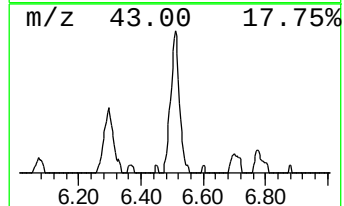
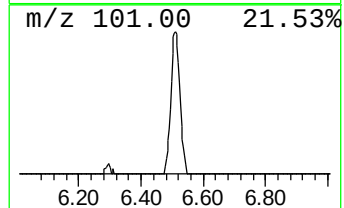
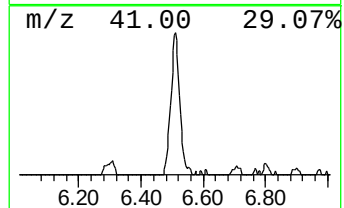
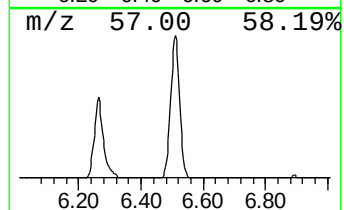
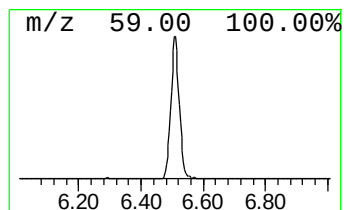
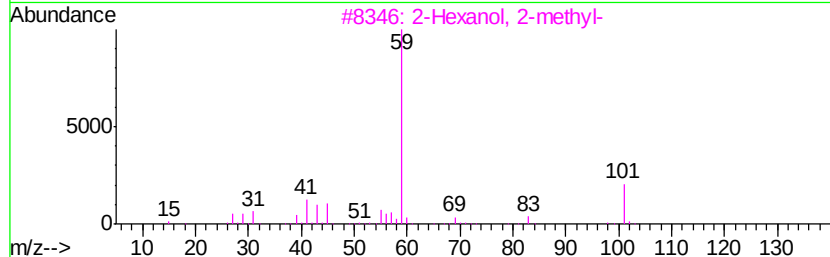
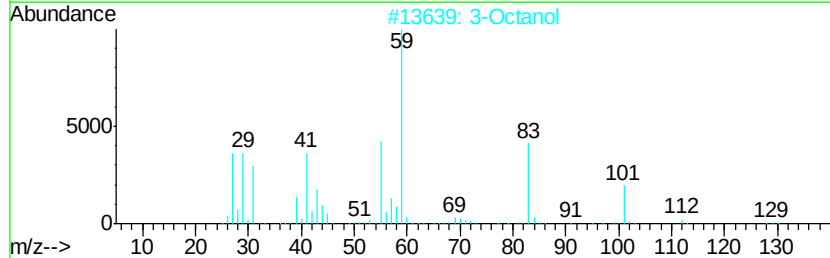
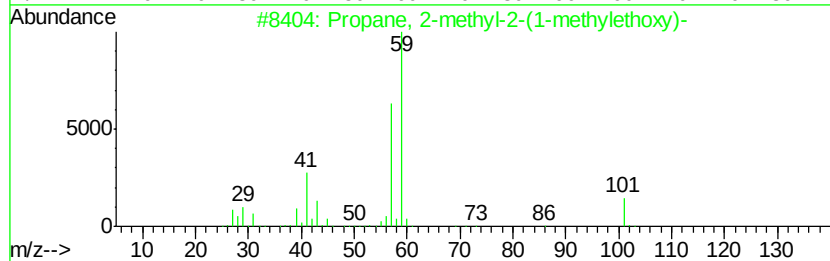
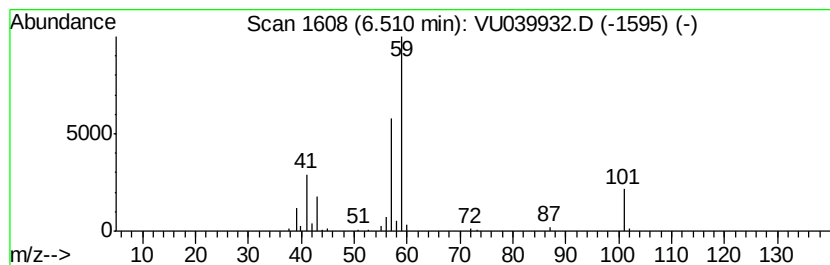
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 3-Octanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	1.99 ug/L	75854	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	83
2		3-Octanol	130	C8H18O	000589-98-0	64
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
4		3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	39
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039932.D
Acq On : 21 Aug 2020 16:50
Operator : SY/MD
Sample : L3776-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y07

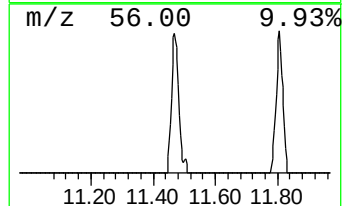
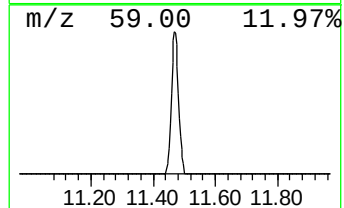
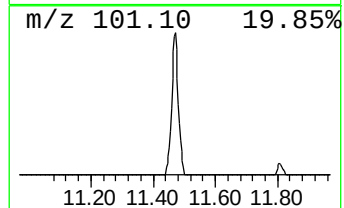
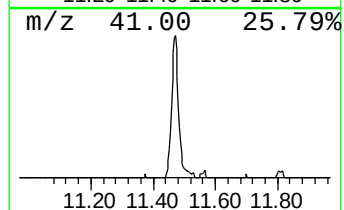
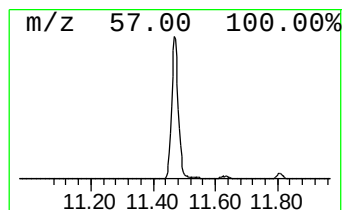
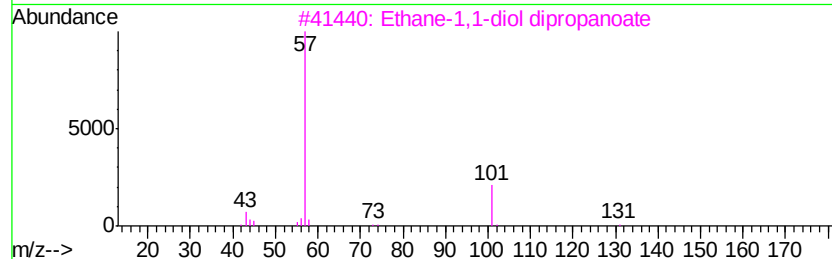
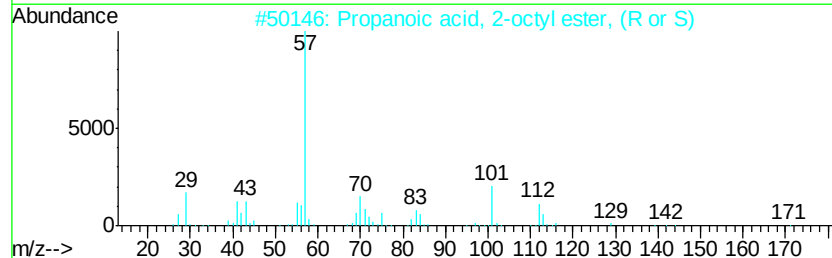
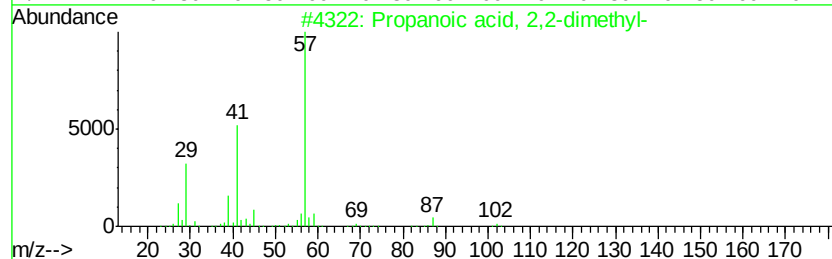
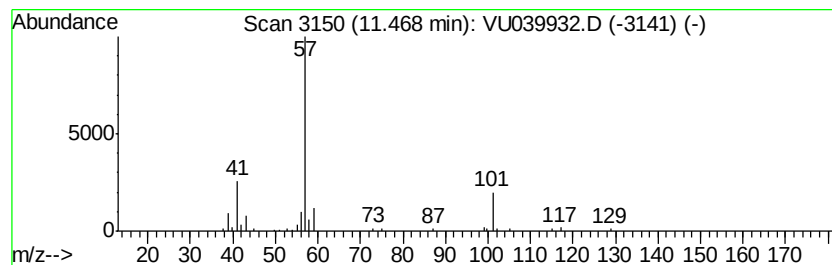
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.47	1.13 ug/L	51677	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-octyl ester, (...)	186	C11H22O2	1000164-41-5	36
3		Ethane-1,1-diol dipropanoate	174	C8H14O4	026880-30-8	33
4		Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	32
5		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	25



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU082120\
Data File : VU039932.D
Acq On : 21 Aug 2020 16:50
Operator : SY/MD
Sample : L3776-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y07

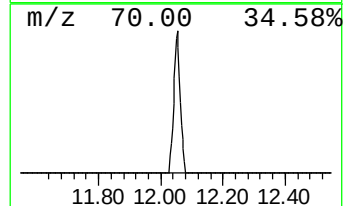
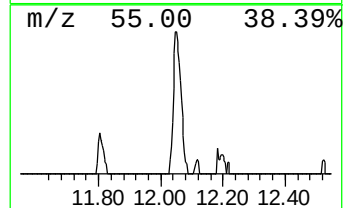
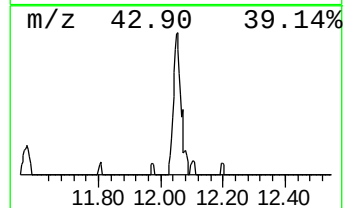
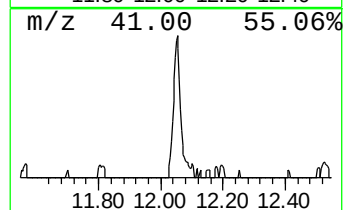
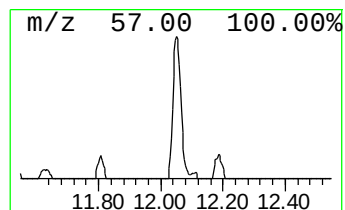
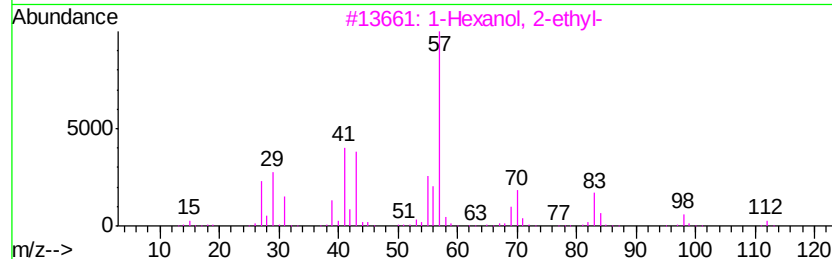
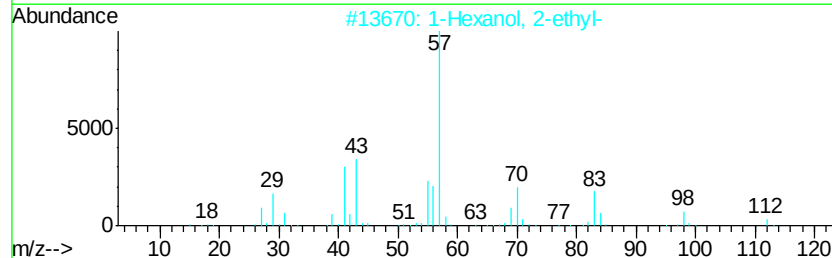
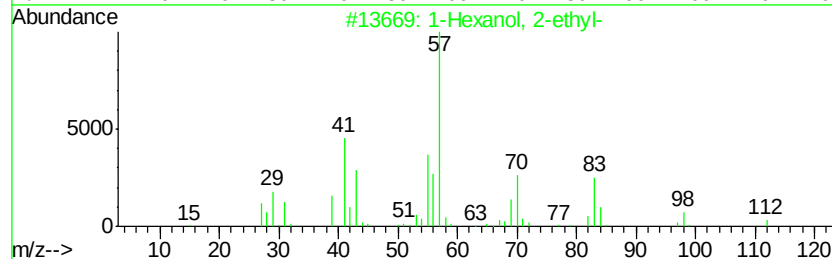
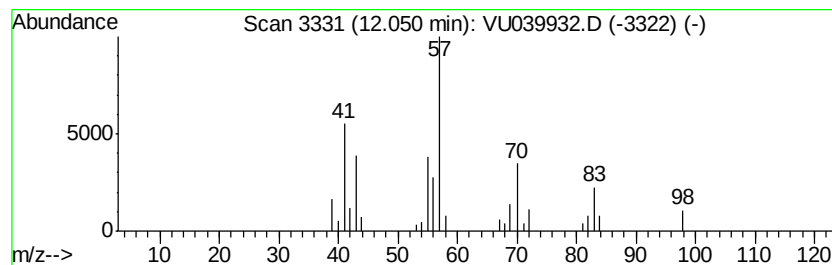
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.05	0.57 ug/L	26312	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	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU082120\
Data File : VU039932.D
Acq On : 21 Aug 2020 16:50
Operator : SY/MD
Sample : L3776-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y07

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR081920WMA.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
Ethane, 1,1-diflu...	1.36	0.6	ug/L	21865	1	6.26	190367	5.0
Isopropyl Alcohol	2.85	8.4	ug/L	321597	1	6.26	190367	5.0
Propane, 2-ethoxy...	4.53	3.2	ug/L	120292	1	6.26	190367	5.0
Ethyl Acetate	4.83	1.2	ug/L	44790	1	6.26	190367	5.0
Propane, 2-methyl...	5.60	1.4	ug/L	54589	1	6.26	190367	5.0
3-Octanol	6.51	2.0	ug/L	75854	1	6.26	190367	5.0
unknown-01	11.47	1.1	ug/L	51677	3	11.81	229202	5.0
1-Hexanol, 2-ethyl-	12.05	0.6	ug/L	26312	3	11.81	229202	5.0