

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
 Data File : VU040089.D
 Acq On : 10 Sep 2020 18:24
 Operator : SY/MD
 Sample : L3961-08
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4Y32

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	1.604	71	82	93	rVB2	56735	88921	15.36%	1.689%
2	1.803	115	144	145	rBV2	50908	194269	33.56%	3.689%
3	1.922	177	181	197	rVB	44003	65270	11.27%	1.239%
4	2.253	280	284	295	rVB4	18270	24982	4.32%	0.474%
5	2.581	374	386	397	rBV	80414	131617	22.73%	2.499%
6	2.652	397	408	438	rVB2	39776	101708	17.57%	1.931%
7	2.832	441	464	524	rBV2	93769	578951	100.00%	10.994%
8	3.234	577	589	602	rBV6	3386	9368	1.62%	0.178%
9	3.382	622	635	651	rVB3	9178	23121	3.99%	0.439%
10	3.890	775	793	813	rBV	81982	202943	35.05%	3.854%
11	4.523	976	990	1006	rVB3	10496	25277	4.37%	0.480%
12	4.649	1014	1029	1051	rBV	62034	171471	29.62%	3.256%
13	4.829	1071	1085	1104	rVB2	25958	59054	10.20%	1.121%
14	5.083	1149	1164	1179	rBV	70893	155937	26.93%	2.961%
15	5.597	1312	1324	1338	rBV4	11992	27150	4.69%	0.516%
16	5.742	1347	1369	1376	rBV2	134077	347120	59.96%	6.591%
17	5.790	1376	1384	1405	rVB	235557	499309	86.24%	9.481%
18	6.263	1516	1531	1554	rBV	125420	245329	42.37%	4.659%
19	6.507	1594	1607	1620	rBV2	47990	96338	16.64%	1.829%
20	6.703	1654	1668	1685	rBV2	89157	170892	29.52%	3.245%
21	7.311	1847	1857	1867	rVB5	6149	10692	1.85%	0.203%
22	7.472	1894	1907	1923	rBV2	51861	96448	16.66%	1.831%
23	7.575	1927	1939	1951	rVB	45379	77814	13.44%	1.478%
24	7.726	1970	1986	1996	rBV6	10362	22850	3.95%	0.434%
25	7.906	2016	2042	2056	rBV	158326	290735	50.22%	5.521%
26	8.185	2112	2129	2141	rBV2	29173	52293	9.03%	0.993%
27	8.430	2191	2205	2214	rBV5	5304	9494	1.64%	0.180%
28	8.504	2219	2228	2239	rVB4	3042	5967	1.03%	0.113%
29	8.639	2255	2270	2291	rBV	235255	420414	72.62%	7.983%
30	8.928	2347	2360	2376	rBV2	8274	16666	2.88%	0.316%
31	9.346	2482	2490	2501	rVB4	3954	5869	1.01%	0.111%
32	9.420	2501	2513	2529	rBV	186001	308960	53.37%	5.867%
33	10.754	2917	2928	2943	rBV	69260	111526	19.26%	2.118%
34	11.471	3142	3151	3161	rBV2	15422	25141	4.34%	0.477%

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ClientSampleId :
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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	11.809	3243	3256	3270	rBV	174542	277784	47.98%	5.275%
36	12.053	3320	3332	3344	rBV2	31263	52433	9.06%	0.996%
37	12.188	3361	3374	3389	rVB	163597	262121	45.28%	4.977%

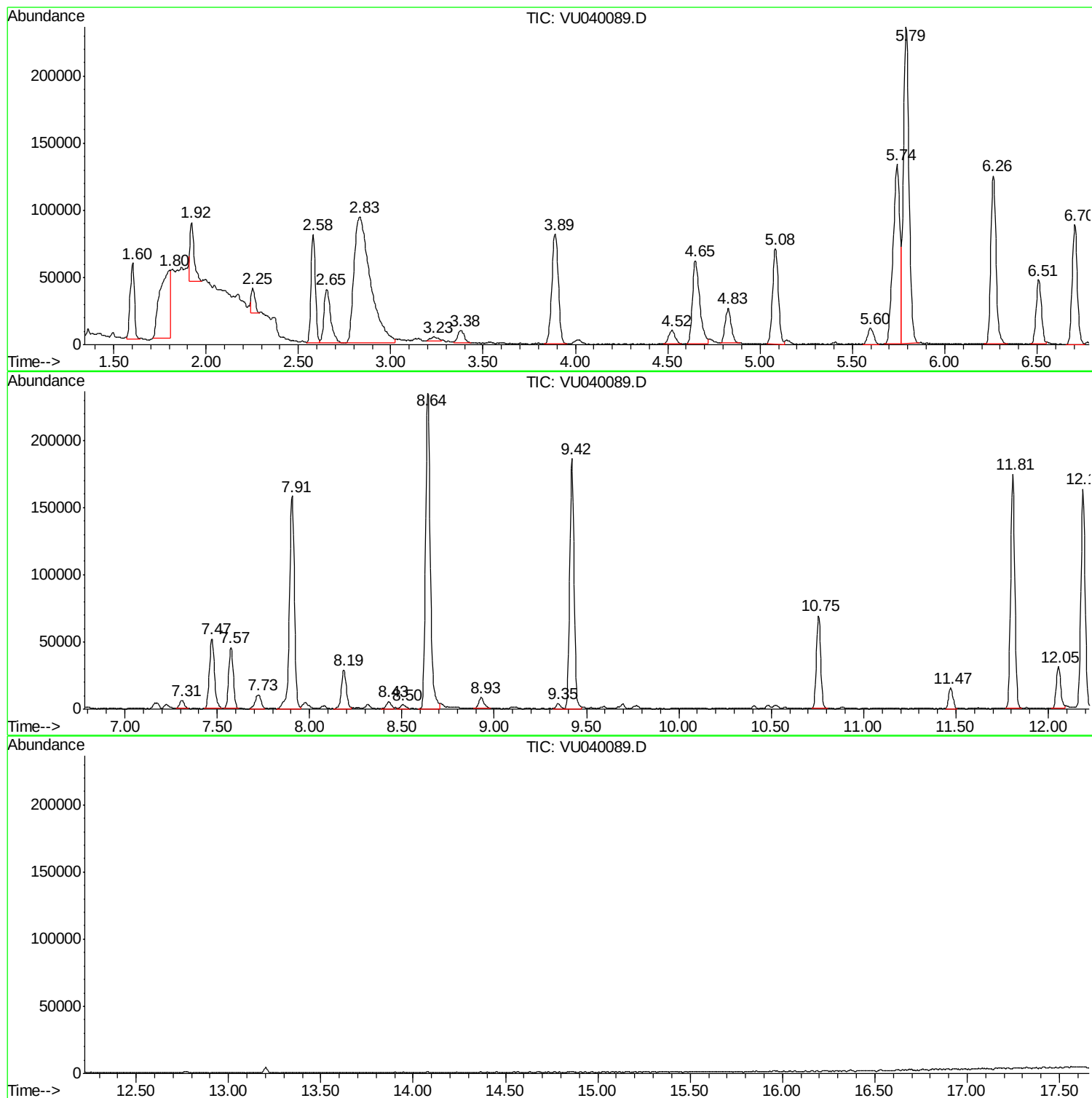
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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



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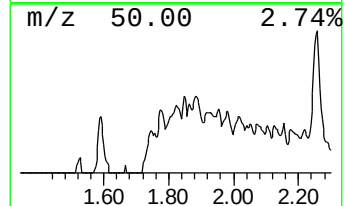
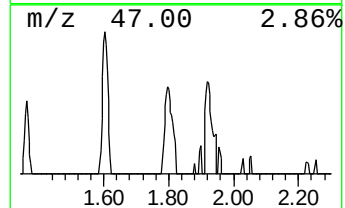
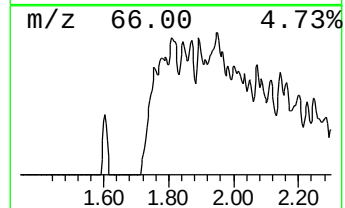
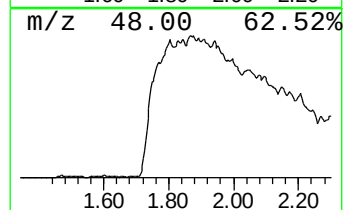
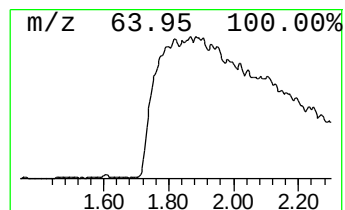
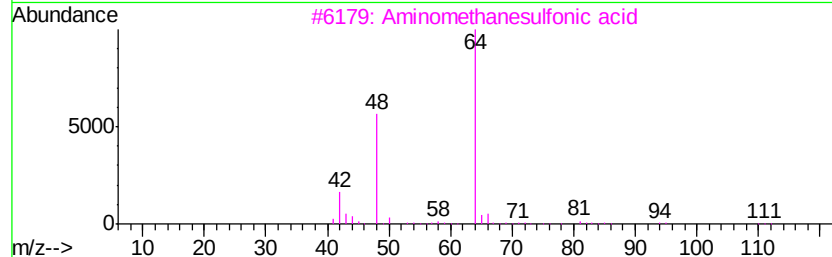
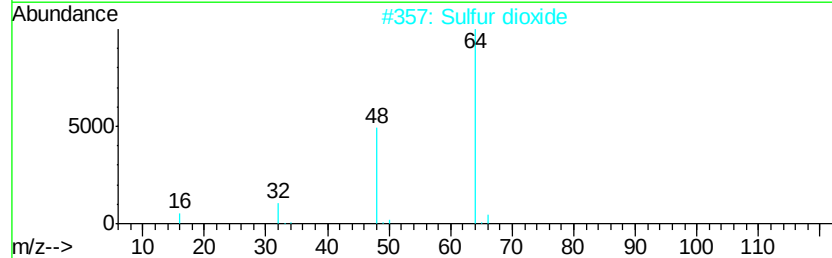
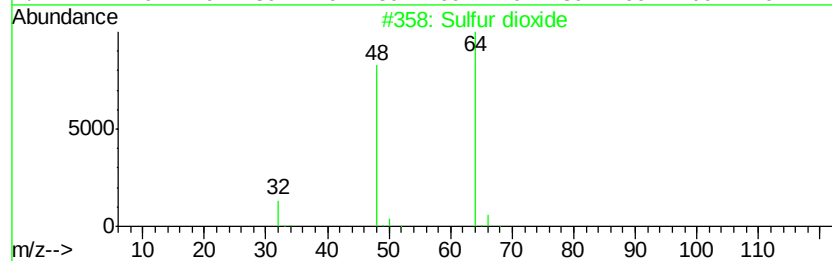
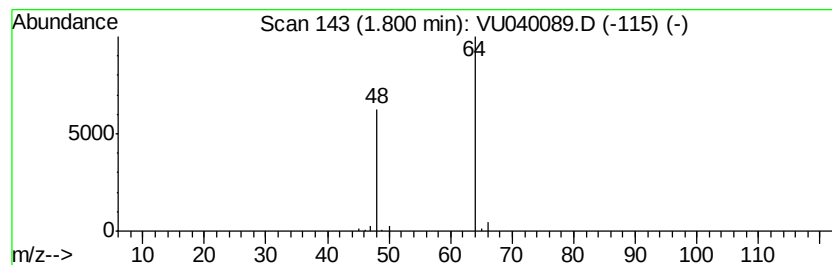
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.80	3.96 ug/L	194269	1,4-Difluorobenzene	6.26
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Sulfur dioxide	64 02S	007446-09-5	83
2	Sulfur dioxide	64 02S	007446-09-5	83
3	Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9	64
4	Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9	64
5	Aminomethanesulfonic acid	111 CH5NO3S	013881-91-9	9



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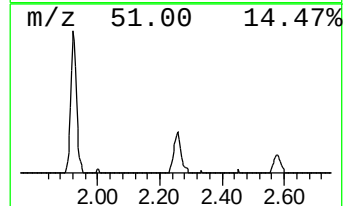
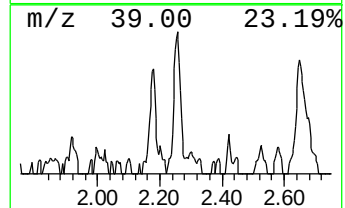
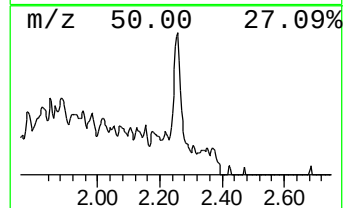
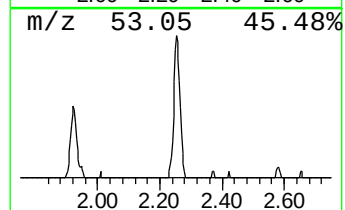
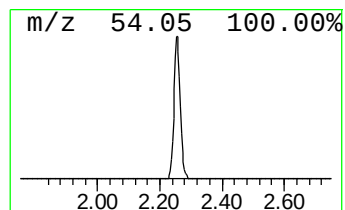
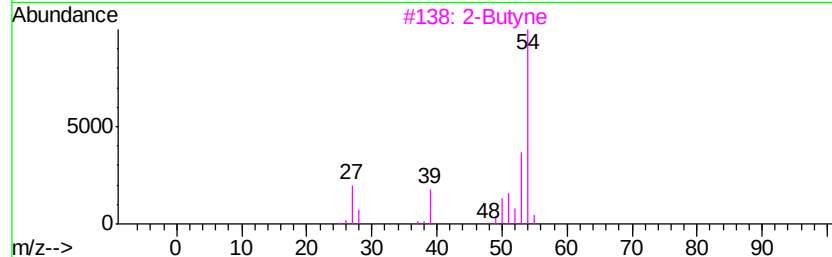
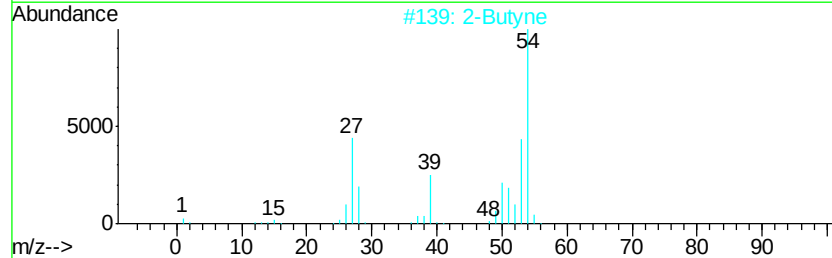
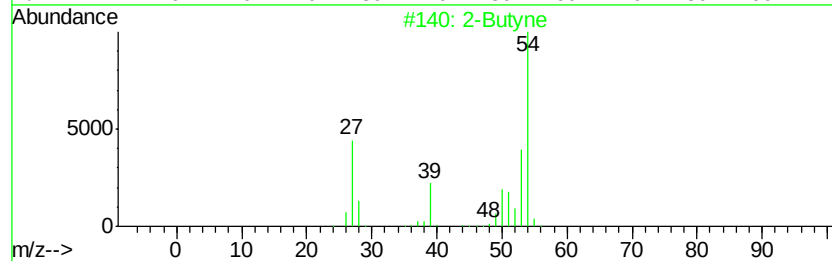
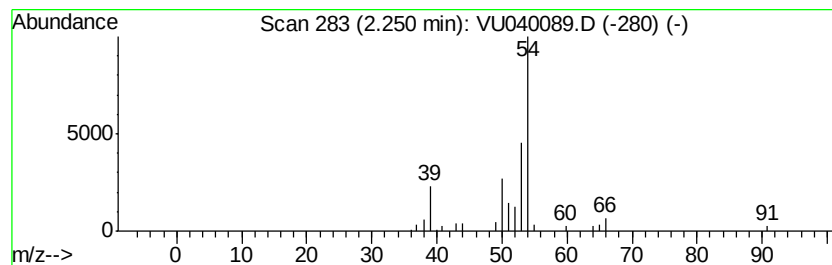
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 2-Butyne Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	0.51 ug/L	24982	1,4-Difluorobenzene	6.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butyne		54	C4H6	000503-17-3	86
2	2-Butyne		54	C4H6	000503-17-3	86
3	2-Butyne		54	C4H6	000503-17-3	86
4	2,5-Dihydrothiophene sulfone		118	C4H6O2S	000077-79-2	83
5	1,2-Butadiene		54	C4H6	000590-19-2	78



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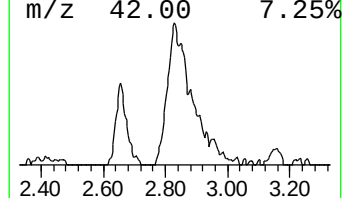
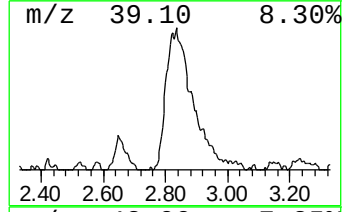
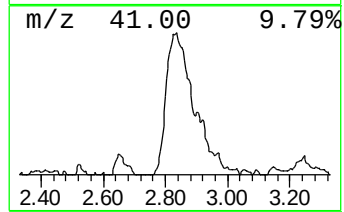
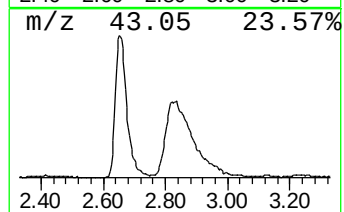
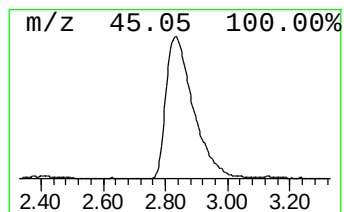
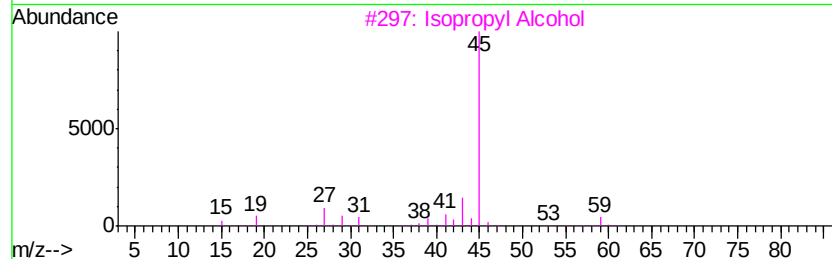
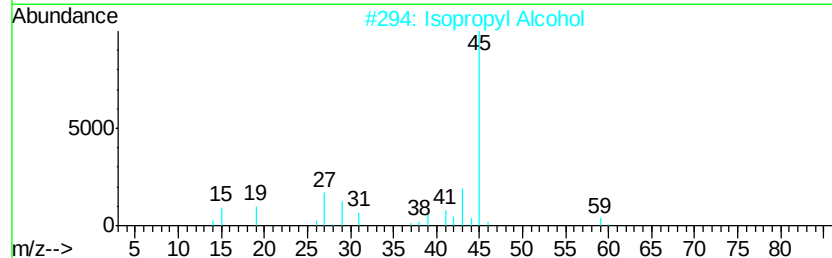
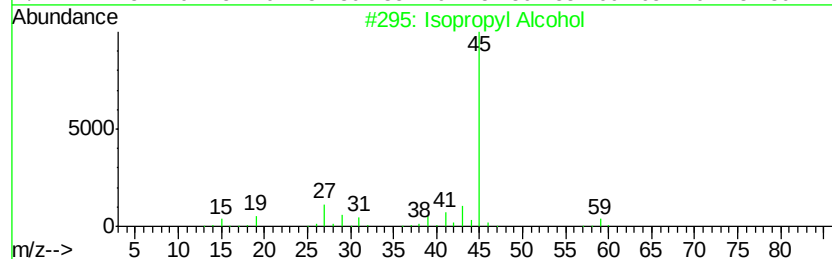
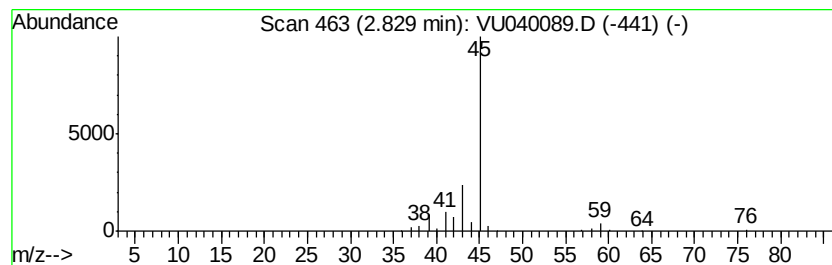
Instrument :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Isopropyl Alcohol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.83	11.80 ug/L	578951	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	78
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
5	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40



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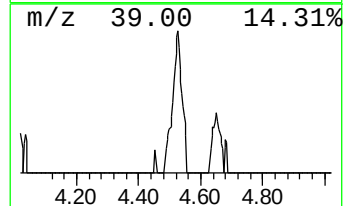
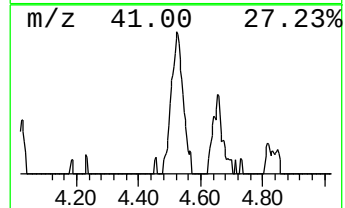
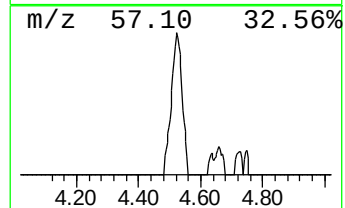
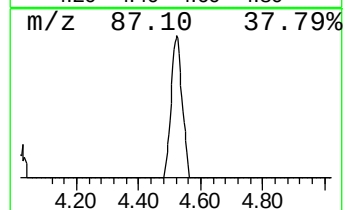
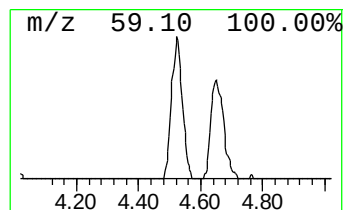
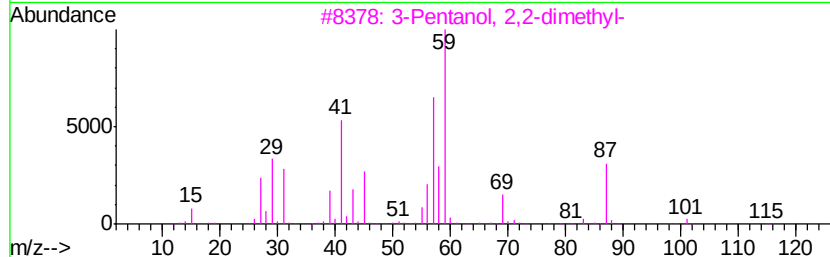
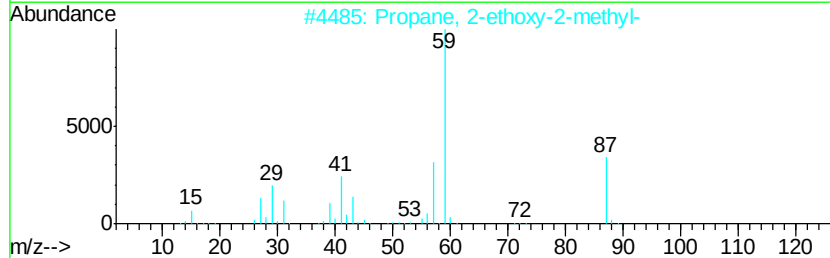
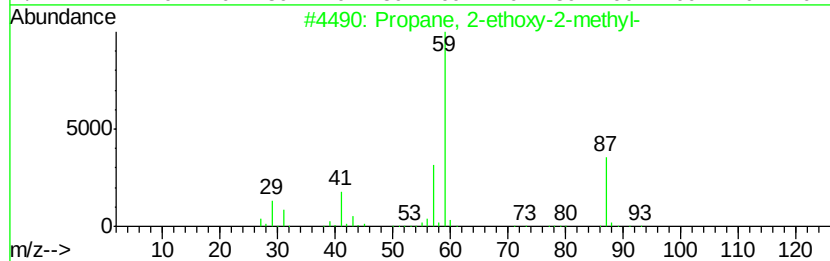
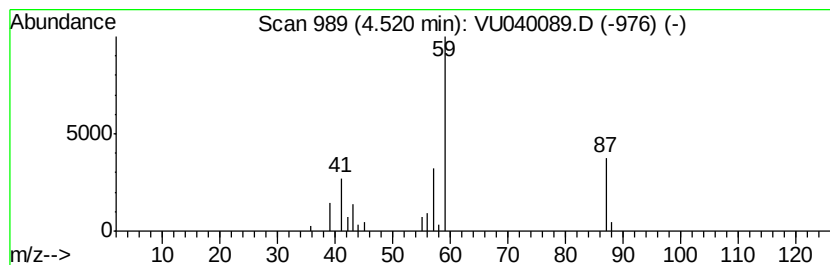
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 Propane, 2-ethoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.52	0.52 ug/L	25277	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	78
2		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
3		3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	39
4		3-Pentanol	88	C5H12O	000584-02-1	36
5		1-Pentanamine	87	C5H13N	000110-58-7	9



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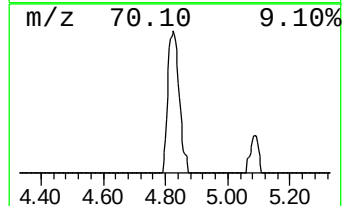
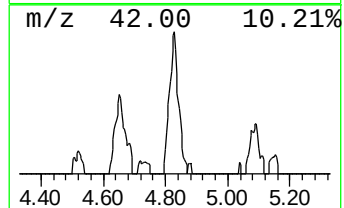
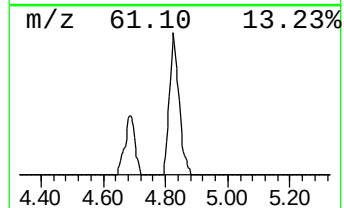
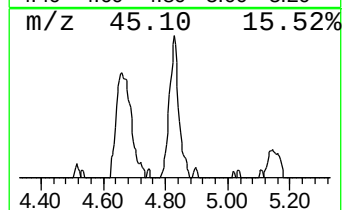
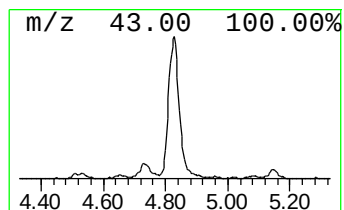
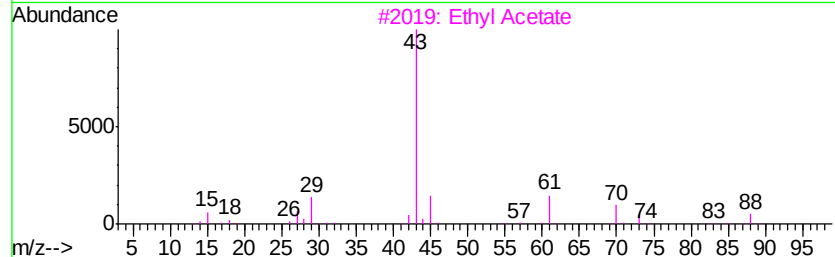
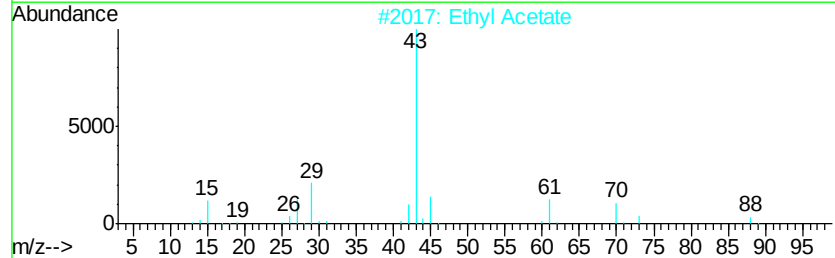
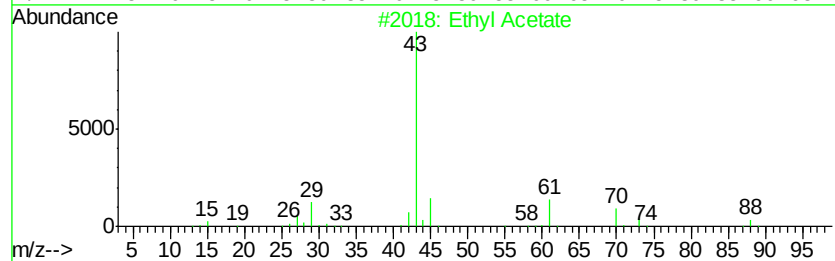
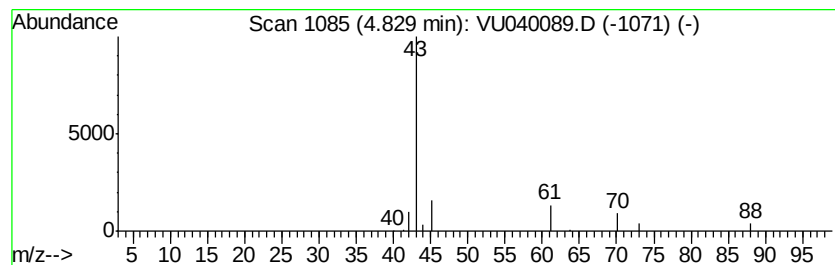
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Ethyl Acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	1.20 ug/L	59054	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	78
4		Ethyl Acetate	88	C4H8O2	000141-78-6	45
5		sec-Butyl nitrite	103	C4H9NO2	000924-43-6	40



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ClientSampleId :
F4Y32

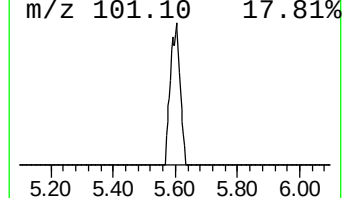
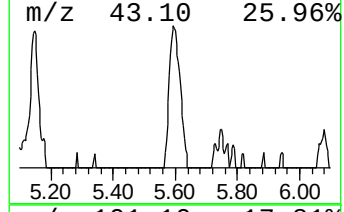
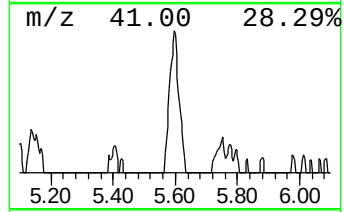
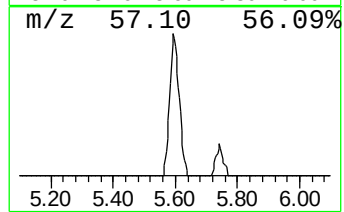
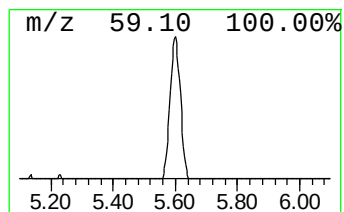
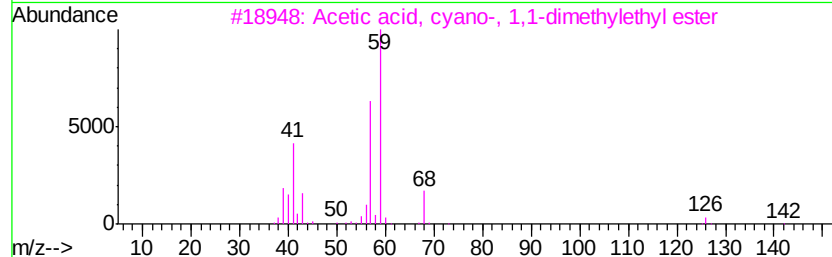
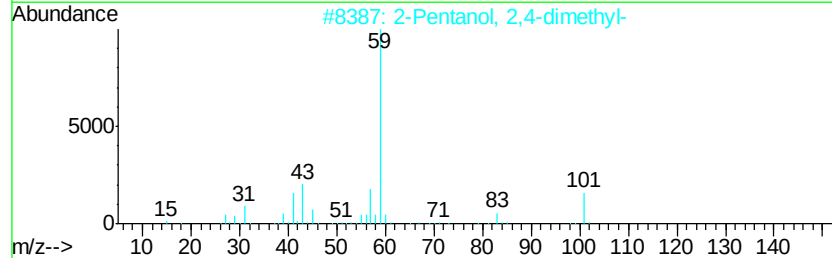
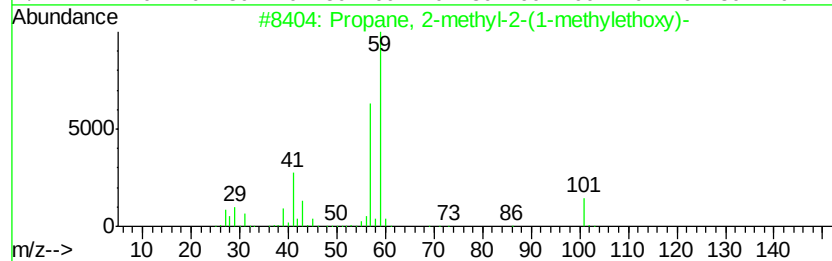
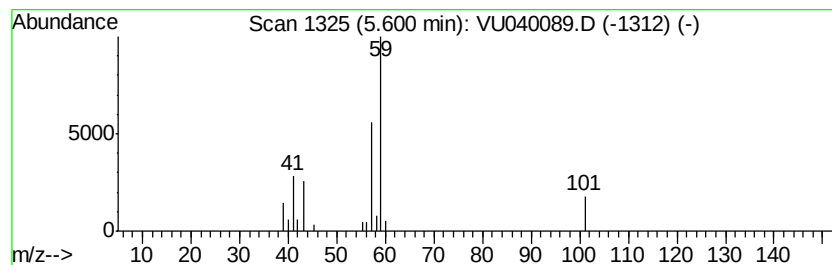
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 Propane, 2-methyl-2-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.60	0.55 ug/L	27150	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	2-Pentanol, 2,4-dimethyl-	116	C7H16O		000625-06-9	74
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2		001116-98-9	56
4	2-Propanol, 2-methyl-	74	C4H10O		000075-65-0	50
5	3-Octanol	130	C8H18O		000589-98-0	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040089.D
Acq On : 10 Sep 2020 18:24
Operator : SY/MD
Sample : L3961-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

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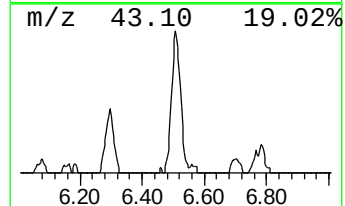
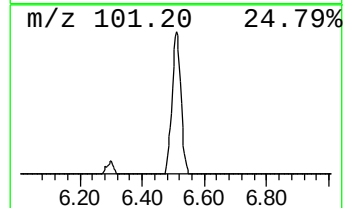
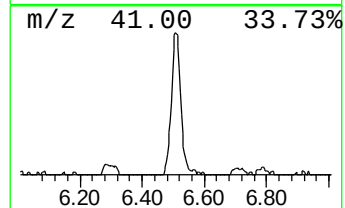
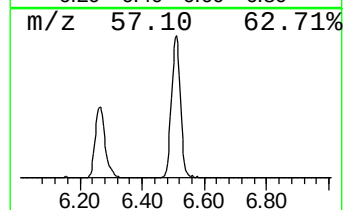
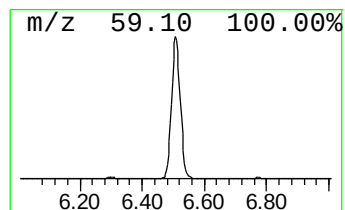
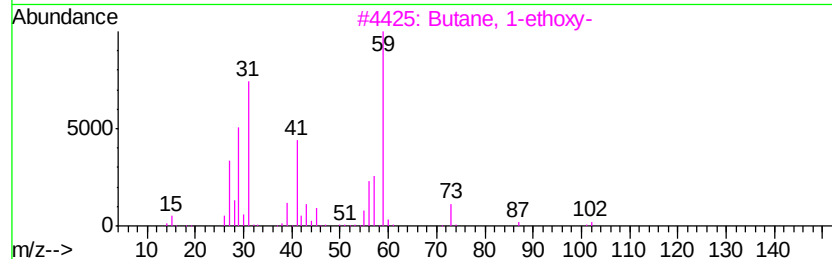
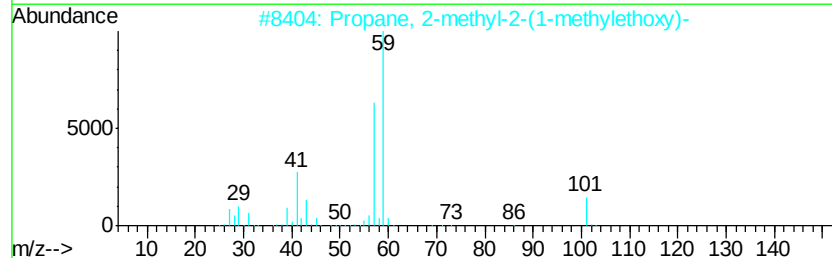
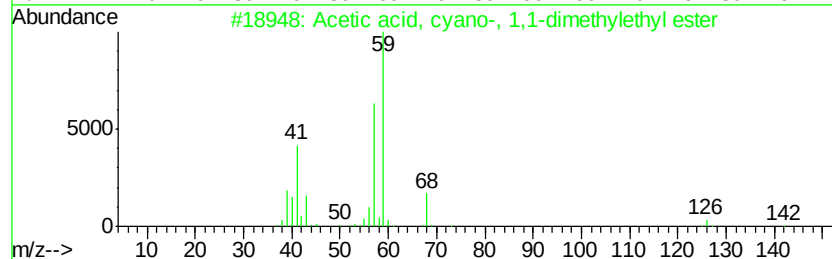
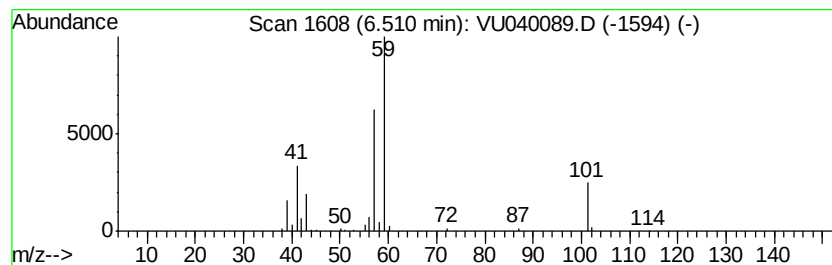
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Acetic acid, cyano-, 1,1-di... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.51	1.96 ug/L	96338	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	56
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	45
4		Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AqO2	007324-58-5	10
5		1-Methyl-3-pyrrolidinol	101	C5H11NO	013220-33-2	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040089.D
Acq On : 10 Sep 2020 18:24
Operator : SY/MD
Sample : L3961-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y32

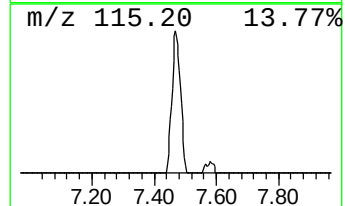
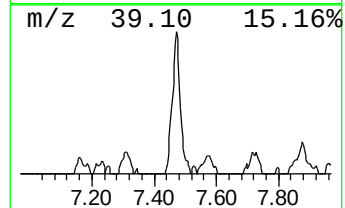
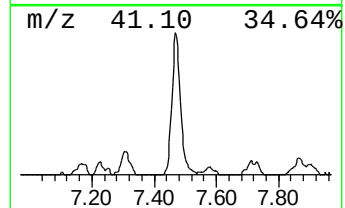
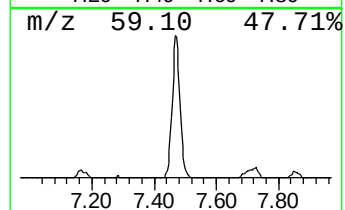
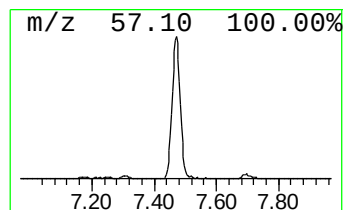
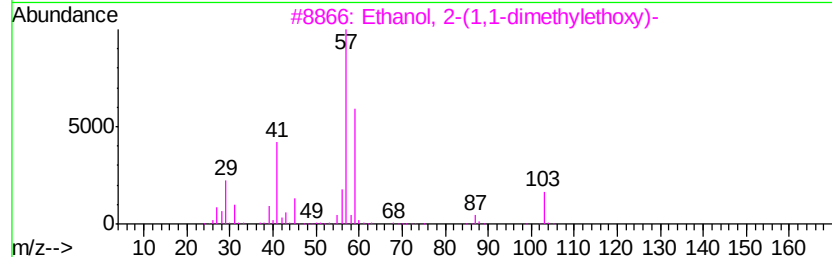
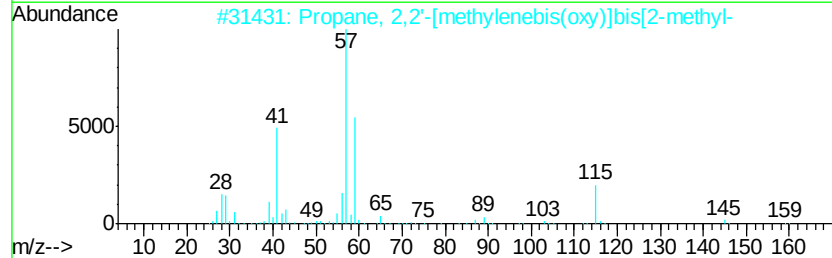
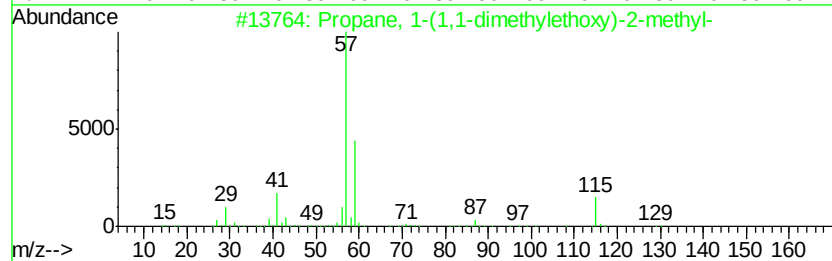
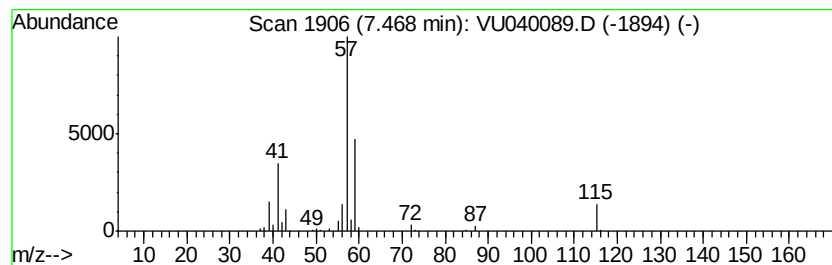
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Propane, 1-(1,1-dimethyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	1.97 ug/L	96448	1,4-Difluorobenzene	6.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-(1,1-dimethylethoxy)-...	130	C8H18O	033021-02-2	78	
2	Propane, 2,2'-[methylenebis(oxy)]...	160	C9H20O2	002568-93-6	74	
3	Ethanol, 2-(1,1-dimethylethoxy)-	118	C6H14O2	007580-85-0	50	
4	tert-Butyl isopropyl carbonate	160	C8H16O3	030221-21-7	39	
5	Propane, 2,2'-[methylenebis(oxy)]...	160	C9H20O2	002568-93-6	39	



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091020\
Data File : VU040089.D
Acq On : 10 Sep 2020 18:24
Operator : SY/MD
Sample : L3961-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 23 Sample Multiplier: 1

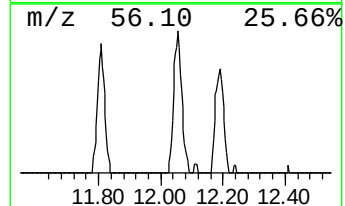
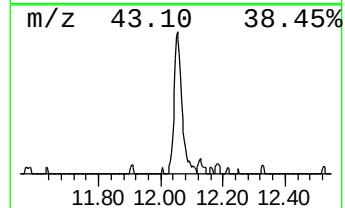
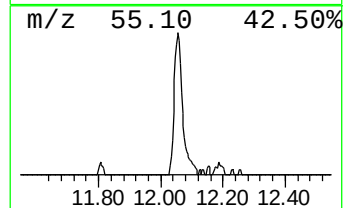
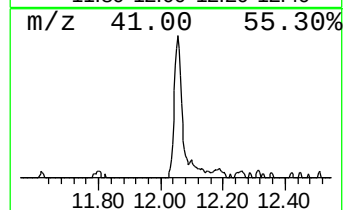
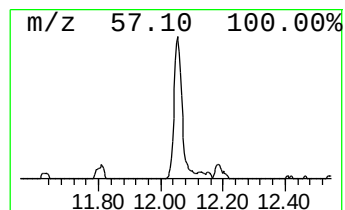
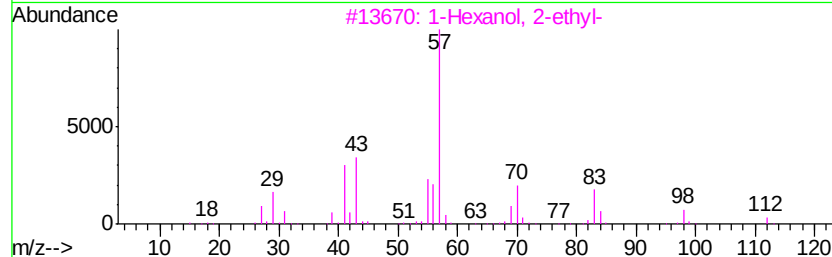
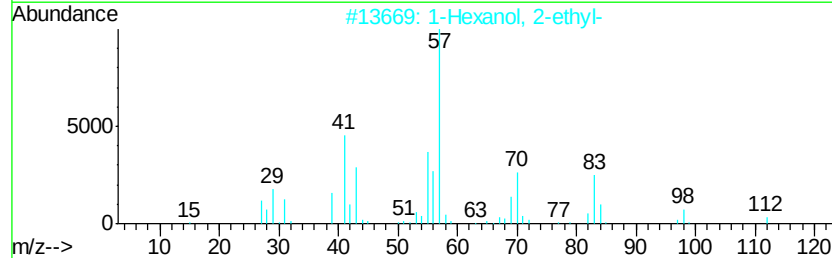
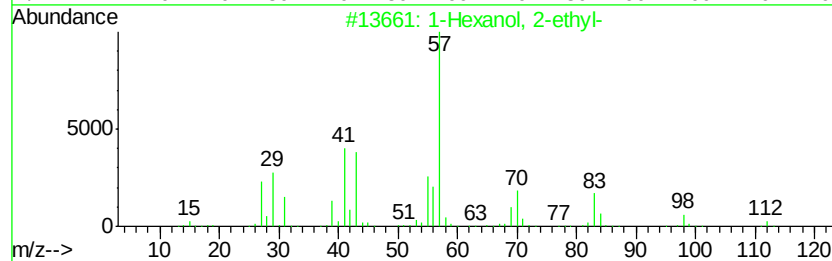
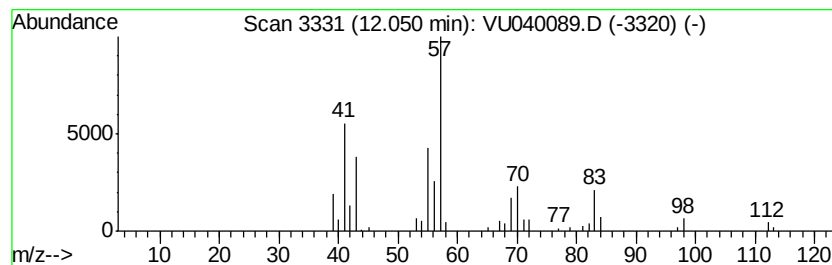
Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR083120WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.05	0.94 ug/L	52433	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	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4	3-Octene, (Z)-	112	C8H16	014850-22-7	50
5	1-Hexene, 3,5-dimethyl-	112	C8H16	007423-69-0	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU091020\
Data File : VU040089.D
Acq On : 10 Sep 2020 18:24
Operator : SY/MD
Sample : L3961-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F4Y32

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
Sulfur dioxide	1.80	4.0	ug/L	194269	1	6.26	245329	5.0
2-Butyne	2.25	0.5	ug/L	24982	1	6.26	245329	5.0
Isopropyl Alcohol	2.83	11.8	ug/L	578951	1	6.26	245329	5.0
Propane, 2-ethoxy...	4.52	0.5	ug/L	25277	1	6.26	245329	5.0
Ethyl Acetate	4.83	1.2	ug/L	59054	1	6.26	245329	5.0
Propane, 2-methyl...	5.60	0.6	ug/L	27150	1	6.26	245329	5.0
Acetic acid, cyan...	6.51	2.0	ug/L	96338	1	6.26	245329	5.0
Propane, 1-(1,1-d...	7.47	2.0	ug/L	96448	1	6.26	245329	5.0
1-Hexanol, 2-ethyl-	12.05	0.9	ug/L	52433	3	11.81	277784	5.0