

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062220\
 Data File : VU039019.D
 Acq On : 22 Jun 2020 21:11
 Operator : SY/MD
 Sample : L3061-08
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXJ5

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\SOMUTR062220WMA.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	40	48	60	rBV	203652	405028	8.14%	1.862%
2	1.610	78	84	96	rVB2	238128	287679	5.78%	1.322%
3	1.948	176	189	203	rVB2	722259	1074239	21.58%	4.938%
4	2.588	376	388	403	rBV2	287779	484580	9.73%	2.228%
5	2.816	448	459	484	rVB3	27677	82213	1.65%	0.378%
6	3.231	569	588	624	rBV	204840	589968	11.85%	2.712%
7	3.909	777	799	823	rBV	2093793	4977823	100.00%	22.883%
8	4.035	824	838	858	rVB2	68045	182247	3.66%	0.838%
9	4.668	1017	1035	1073	rBV2	280595	800871	16.09%	3.682%
10	4.851	1079	1092	1113	rVB2	65897	162637	3.27%	0.748%
11	5.099	1154	1169	1192	rBV	238665	531210	10.67%	2.442%
12	5.758	1349	1374	1389	rBV2	483121	1236465	24.84%	5.684%
13	6.279	1520	1536	1556	rBV	344173	645833	12.97%	2.969%
14	6.594	1616	1634	1653	rVB2	28262	60796	1.22%	0.279%
15	6.719	1658	1673	1690	rBV	305191	588329	11.82%	2.705%
16	6.944	1725	1743	1758	rBV	951833	1850217	37.17%	8.505%
17	7.362	1861	1873	1889	rBV	55110	104564	2.10%	0.481%
18	7.539	1914	1928	1935	rBV2	98948	173982	3.50%	0.800%
19	7.591	1935	1944	1959	rVB	129456	229208	4.60%	1.054%
20	7.739	1973	1990	2006	rBV2	337131	636293	12.78%	2.925%
21	7.922	2033	2047	2062	rBV	576006	992290	19.93%	4.562%
22	8.202	2120	2134	2152	rBV	84600	144982	2.91%	0.666%
23	8.655	2259	2275	2311	rBV	834800	1551342	31.17%	7.132%
24	9.333	2474	2486	2496	rBV2	34543	55600	1.12%	0.256%
25	9.436	2502	2518	2540	rBV	536510	898001	18.04%	4.128%
26	10.276	2766	2779	2799	rBV	299397	626880	12.59%	2.882%
27	10.771	2919	2933	2952	rVB	243994	400635	8.05%	1.842%
28	11.044	3001	3018	3033	rBV2	174278	305930	6.15%	1.406%
29	11.822	3248	3260	3277	rBV	500708	797800	16.03%	3.667%
30	12.205	3366	3379	3396	rBV	547706	875716	17.59%	4.026%

Sum of corrected areas: 21753358

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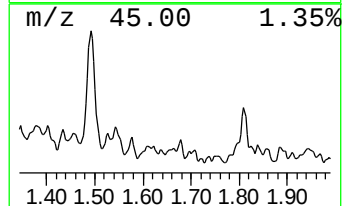
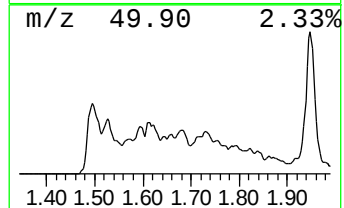
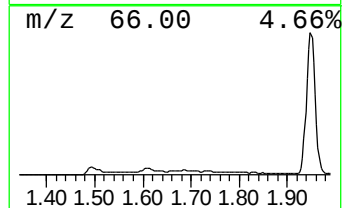
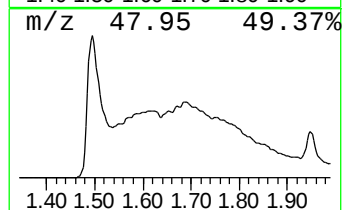
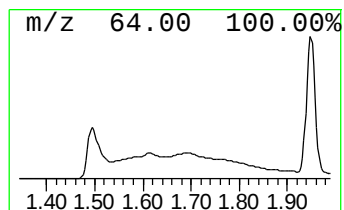
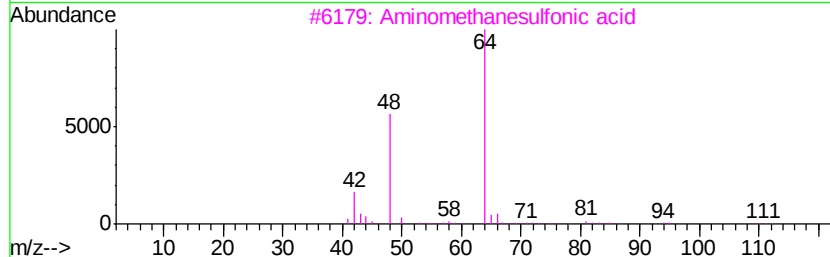
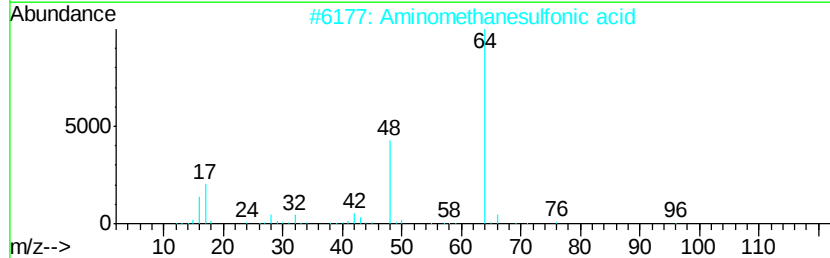
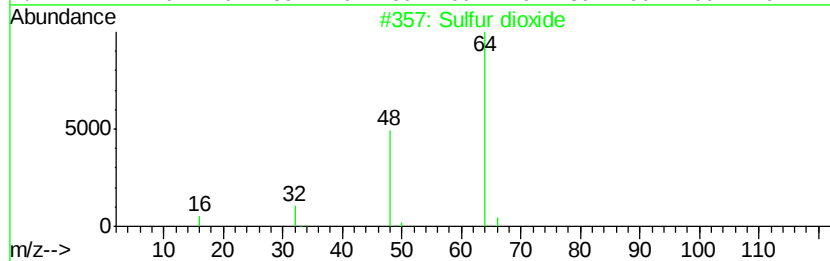
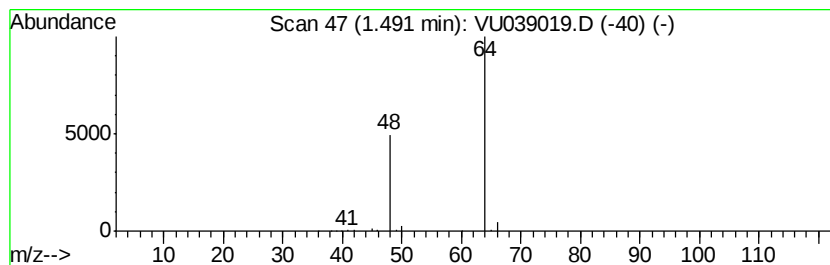
Instrument :
MSVOA_U
ClientSampleId :
BFXJ5

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.49	3.14 ug/L	405028	1,4-Difluorobenzene	6.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7



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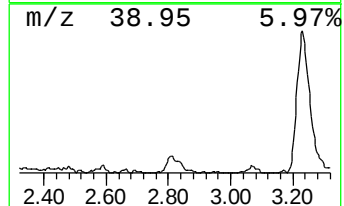
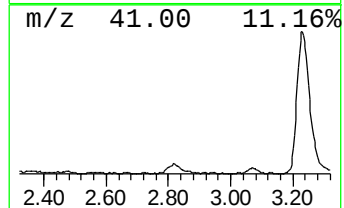
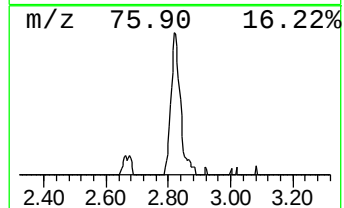
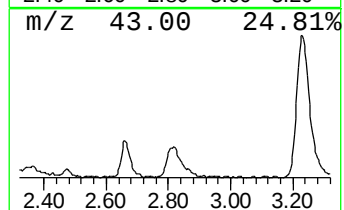
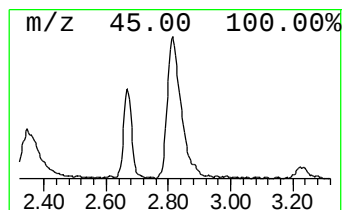
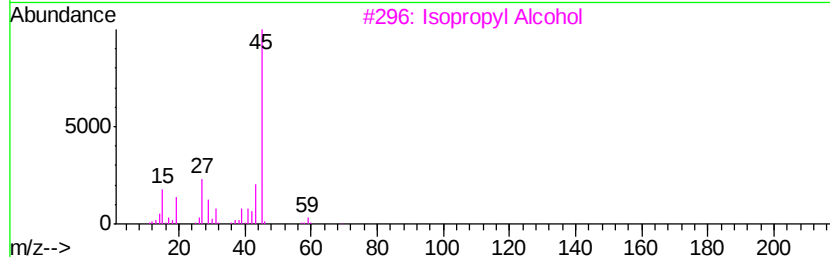
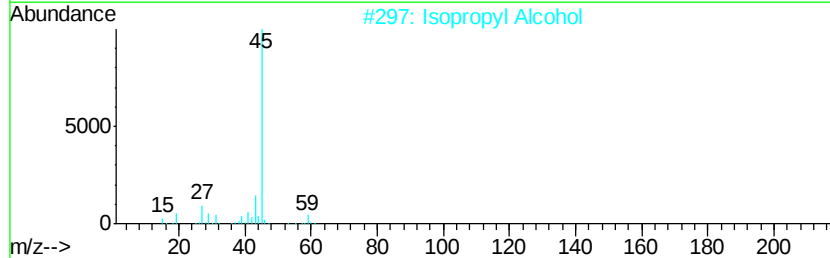
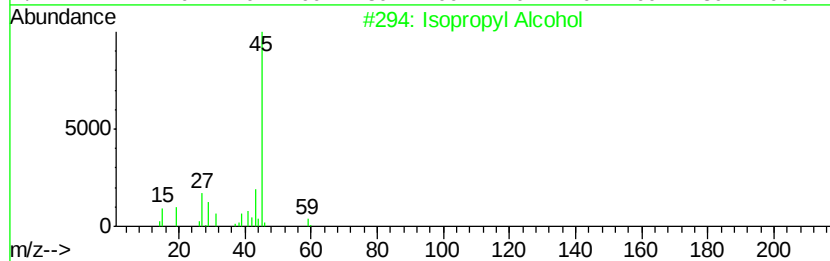
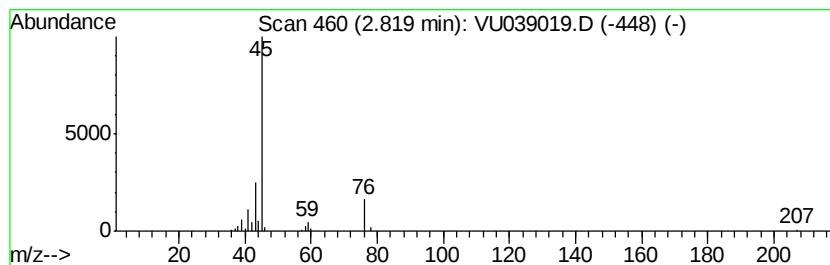
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Isopropyl Alcohol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.82	0.64 ug/L	82213	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	50
4			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	39
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	39



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

Instrument :
MSVOA_U
ClientSampleId :
BFXJ5

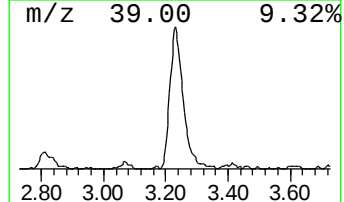
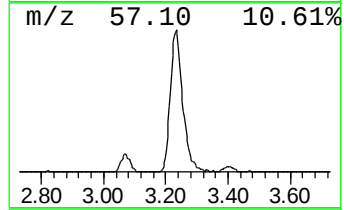
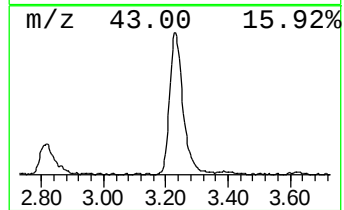
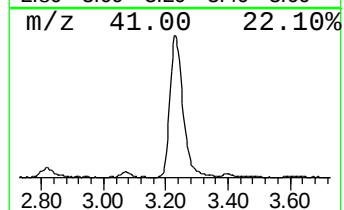
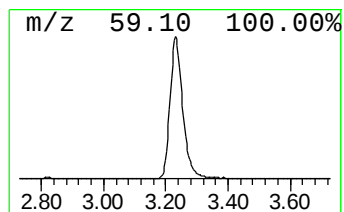
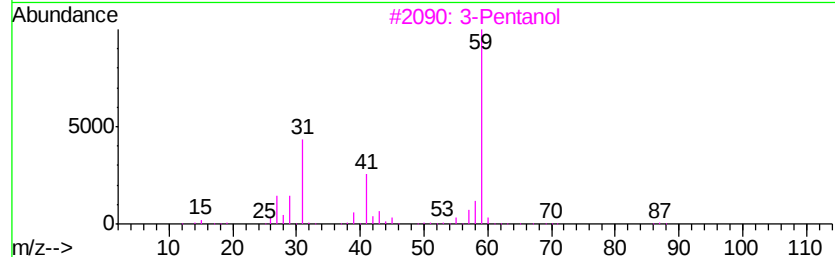
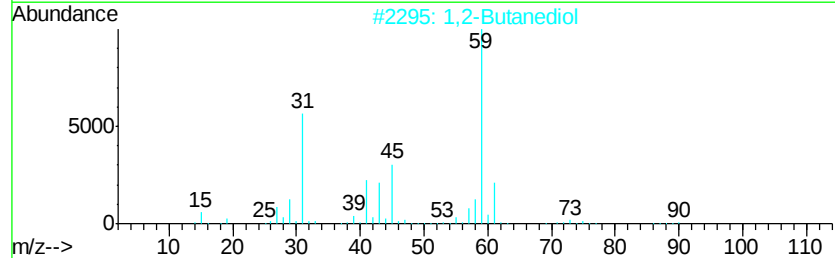
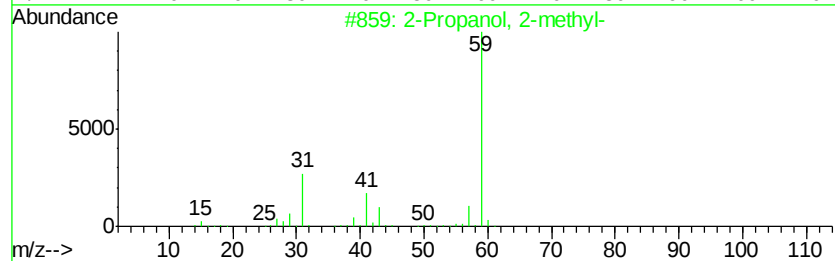
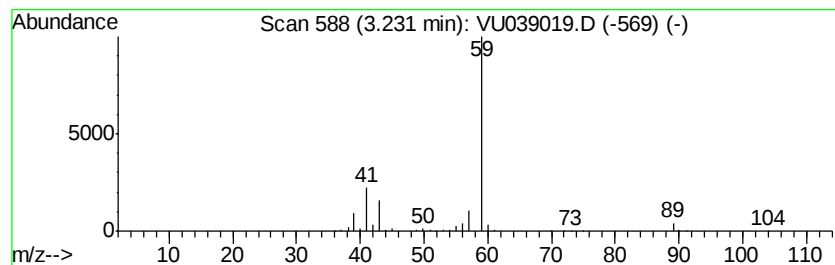
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.23	4.57 ug/L	589968	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	72
2			1,2-Butanediol	90	C4H10O2	000584-03-2	72
3			3-Pentanol	88	C5H12O	000584-02-1	56
4			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	56
5			2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	40



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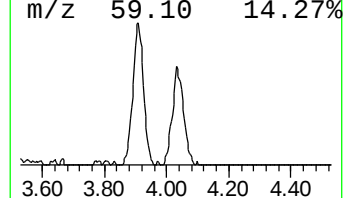
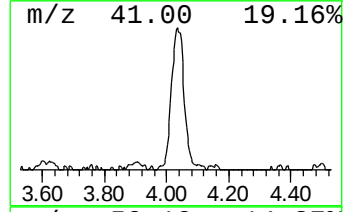
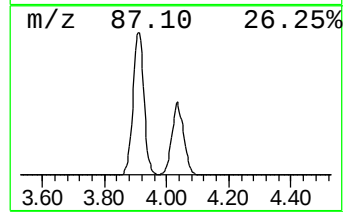
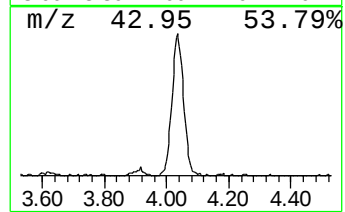
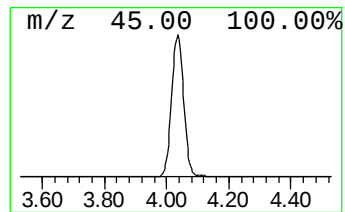
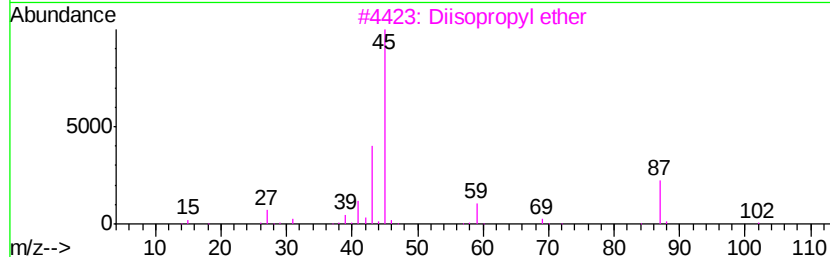
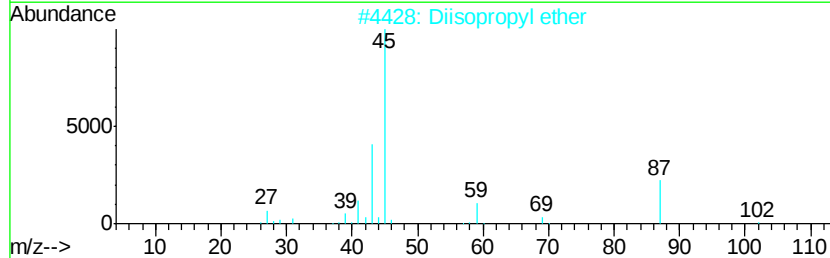
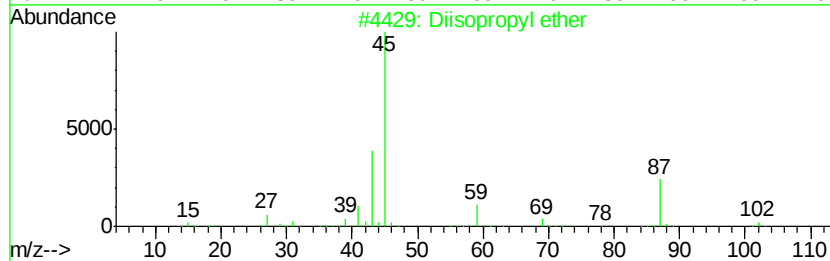
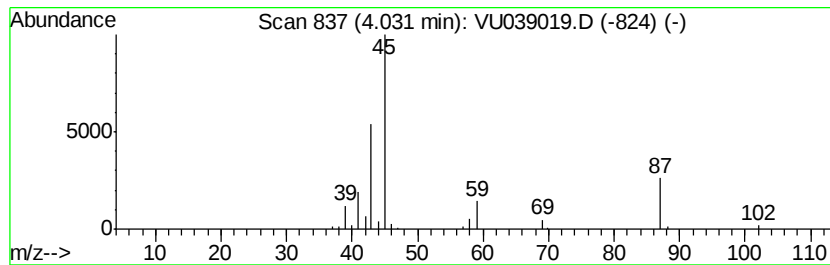
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Diisopropyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.03	1.41 ug/L	182247	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl ether	102	C6H14O	000108-20-3	78
2			Diisopropyl ether	102	C6H14O	000108-20-3	78
3			Diisopropyl ether	102	C6H14O	000108-20-3	78
4			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64
5			Ether, 2-chloro-1-methylethyl is...	136	C6H13ClO	098277-76-0	56



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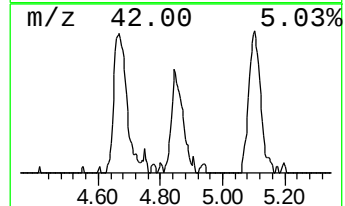
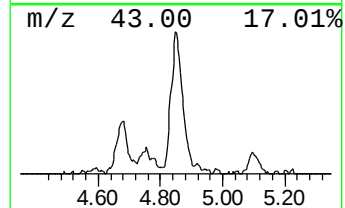
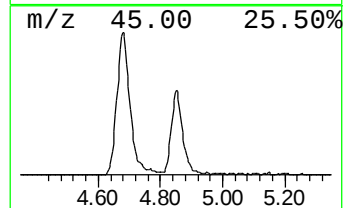
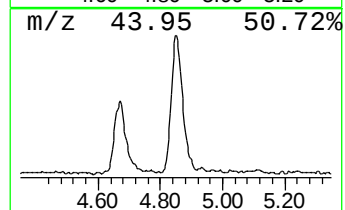
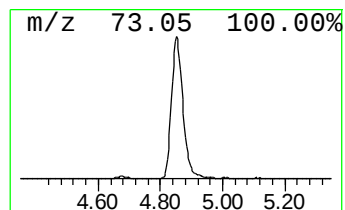
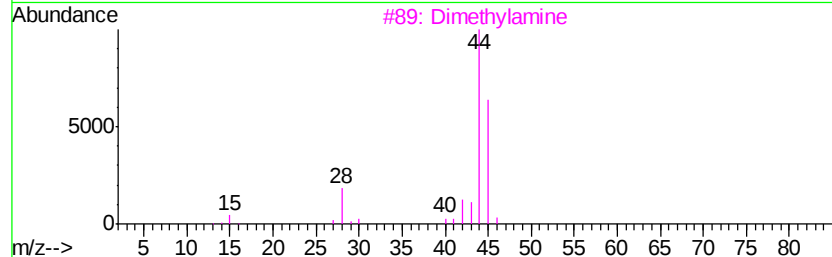
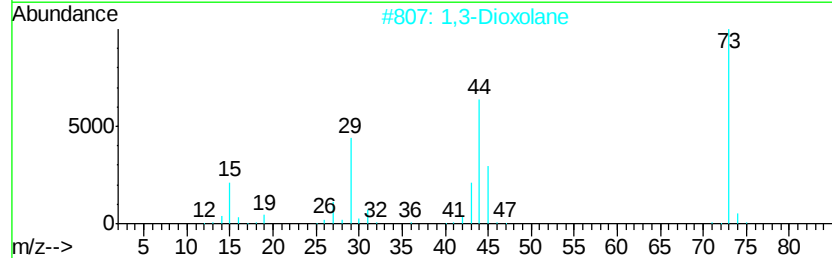
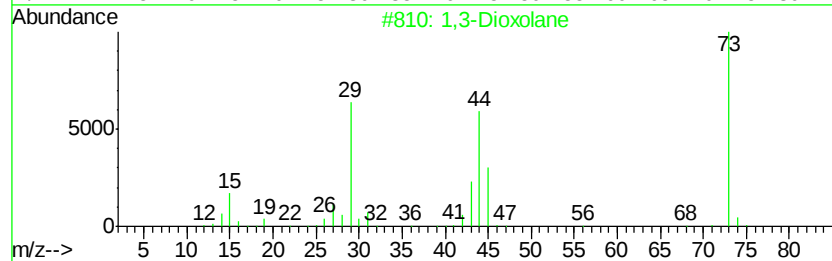
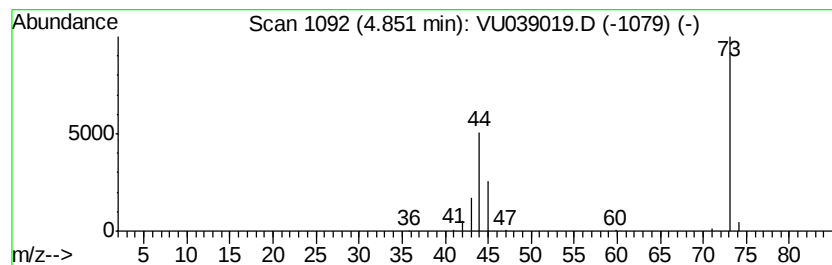
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 1,3-Dioxolane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	1.26 ug/L	162637	1,4-Difluorobenzene	6.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane		74	C3H6O2	000646-06-0	90
2	1,3-Dioxolane		74	C3H6O2	000646-06-0	90
3	Dimethylamine		45	C2H7N	000124-40-3	7
4	N-Ethylformamide		73	C3H7NO	000627-45-2	5
5	Guanidine, methyl-		73	C2H7N3	000471-29-4	5



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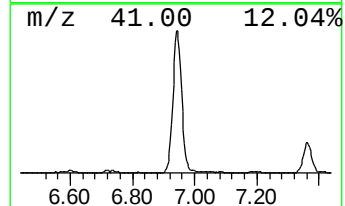
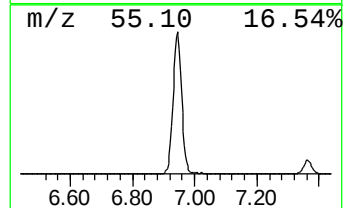
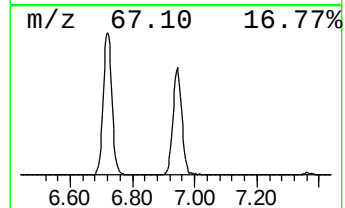
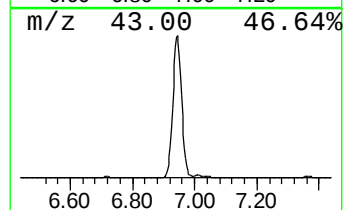
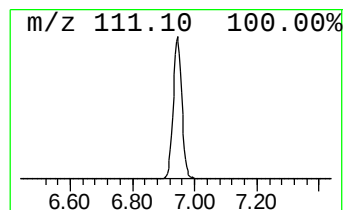
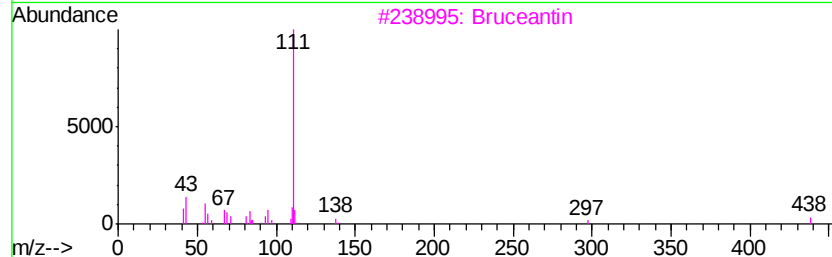
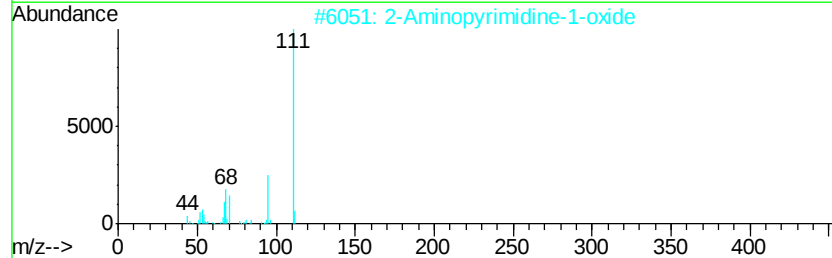
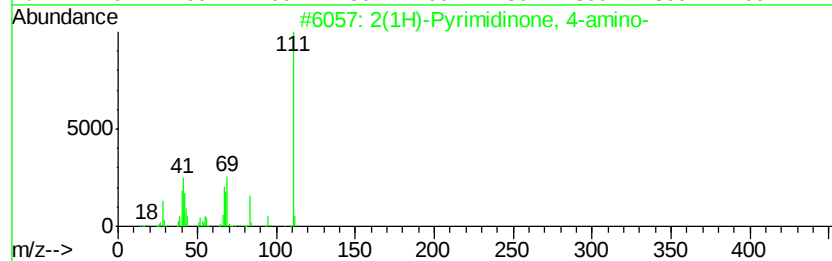
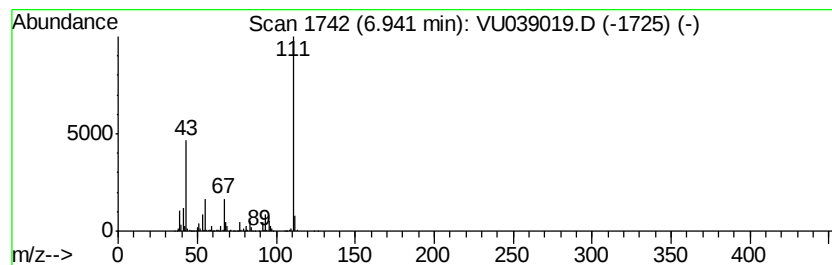
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.94	14.32 ug/L	1850220	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	72
2		2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	64
3		Bruceantin	548	C28H36O11	041451-75-6	50
4		2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	50
5		2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039019.D
Acq On : 22 Jun 2020 21:11
Operator : SY/MD
Sample : L3061-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
BFXJ5

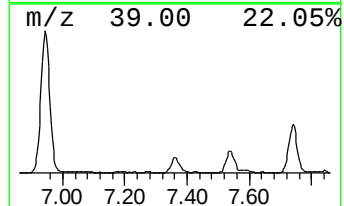
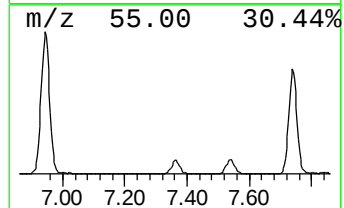
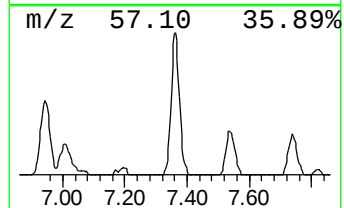
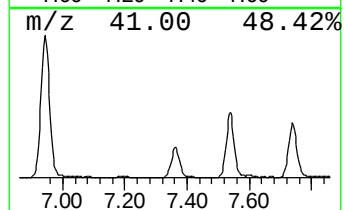
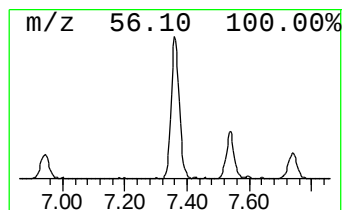
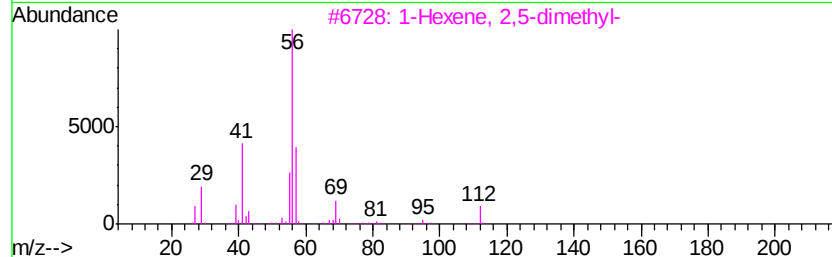
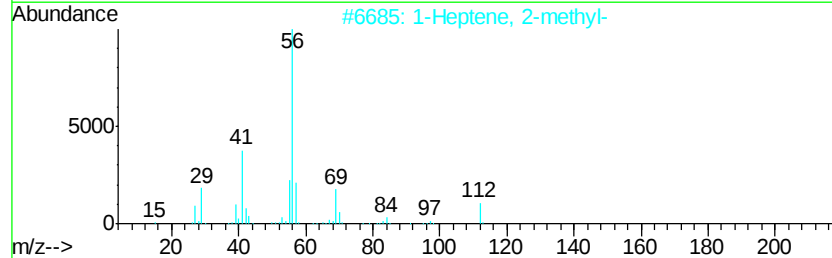
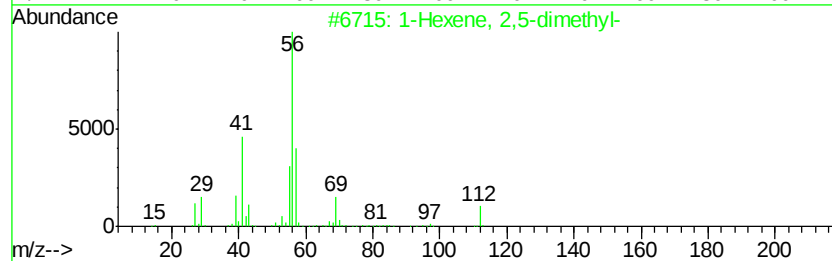
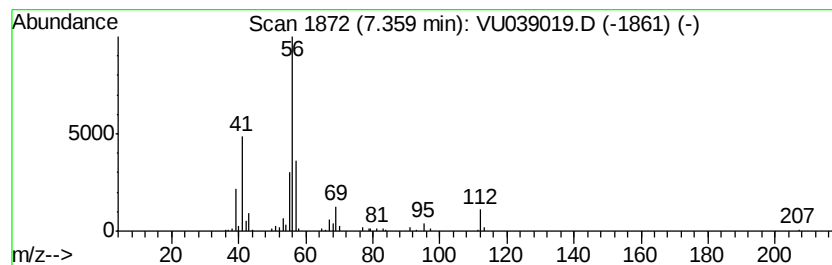
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	0.81 ug/L	104564	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	90
2		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	86
3		1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	80
4		1-Heptene, 2-methyl-	112	C8H16	015870-10-7	72
5		2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039019.D
Acq On : 22 Jun 2020 21:11
Operator : SY/MD
Sample : L3061-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXJ5

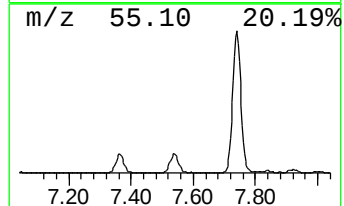
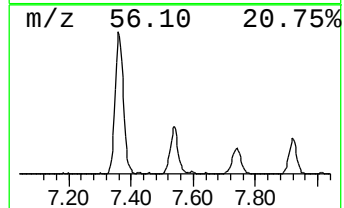
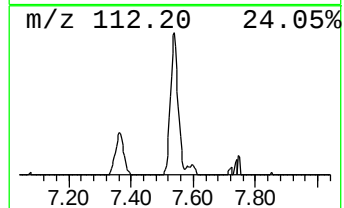
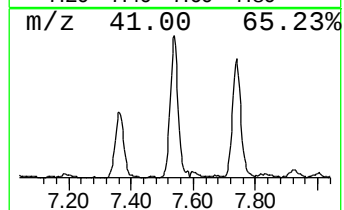
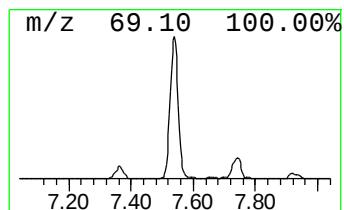
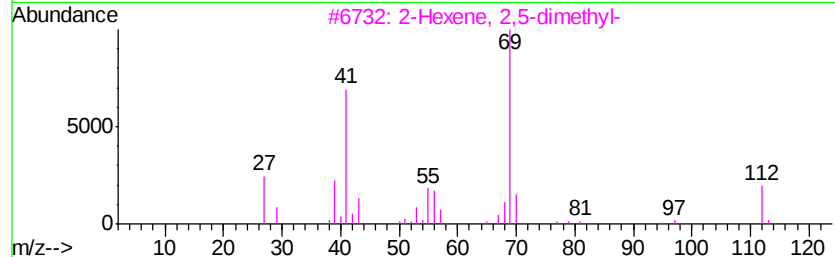
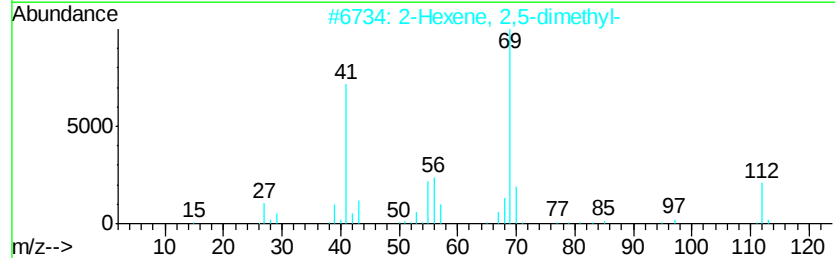
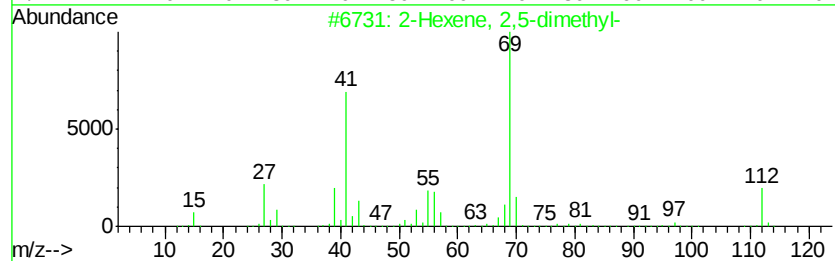
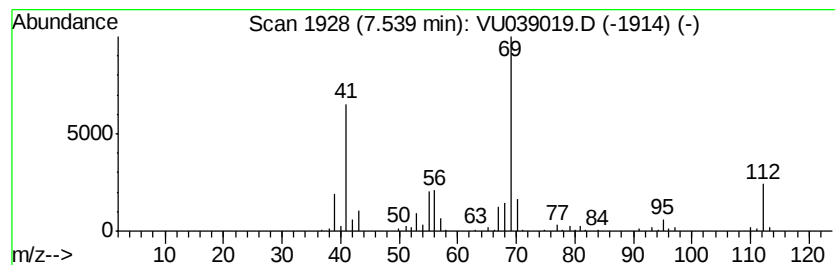
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	1.35 ug/L	173982	1,4-Difluorobenzene	6.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 2,5-dimethyl-		112	C8H16	003404-78-2	90
2	2-Hexene, 2,5-dimethyl-		112	C8H16	003404-78-2	90
3	2-Hexene, 2,5-dimethyl-		112	C8H16	003404-78-2	90
4	2-Hexene, 2,5-dimethyl-		112	C8H16	003404-78-2	87
5	3-Hexene, 2,5-dimethyl-, (E)-		112	C8H16	000692-70-6	83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039019.D
Acq On : 22 Jun 2020 21:11
Operator : SY/MD
Sample : L3061-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

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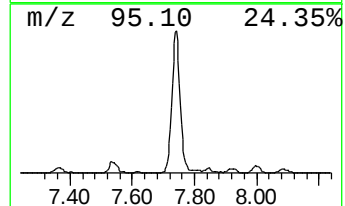
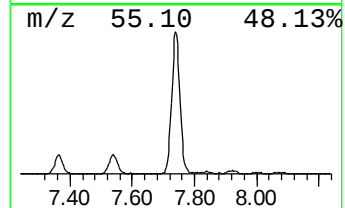
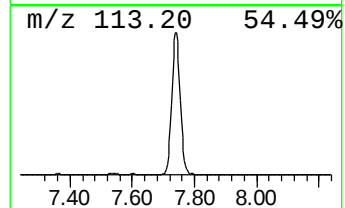
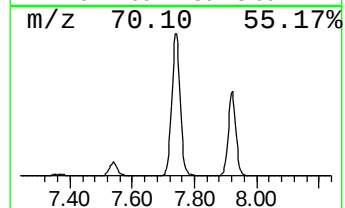
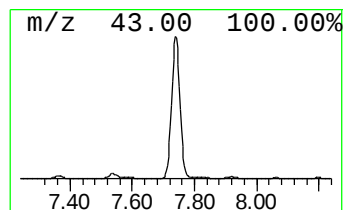
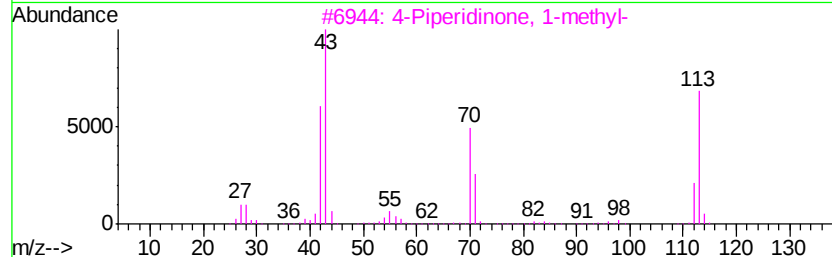
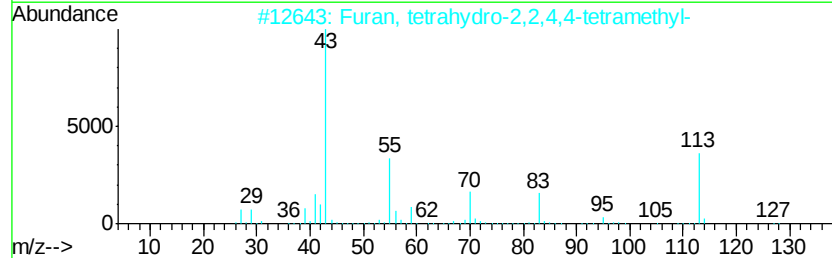
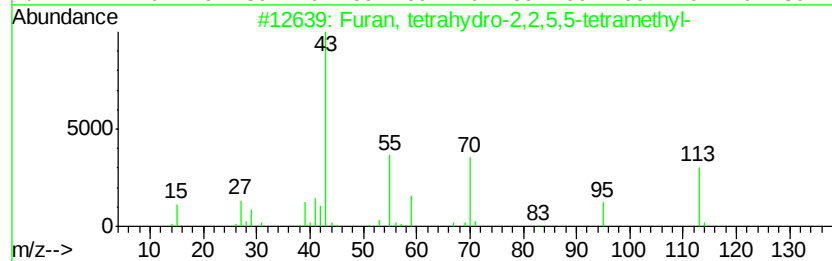
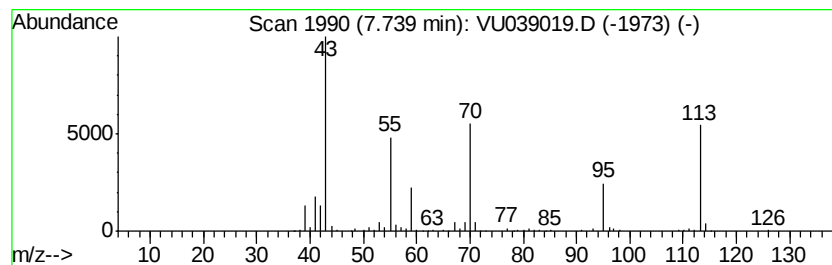
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	4.93 ug/L	636293	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	64		
2	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53		
3	4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50		
4	1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	47		
5	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	45		



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039019.D
Acq On : 22 Jun 2020 21:11
Operator : SY/MD
Sample : L3061-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

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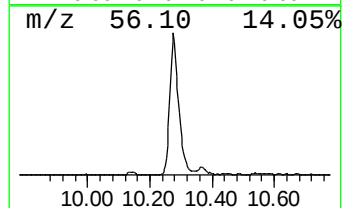
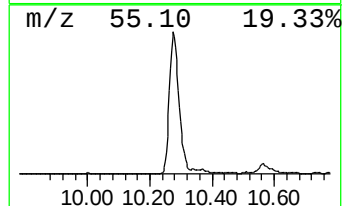
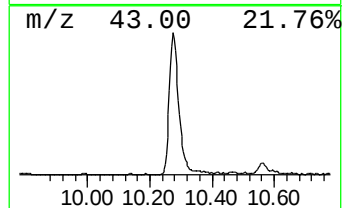
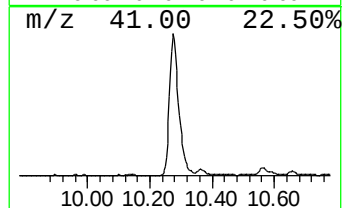
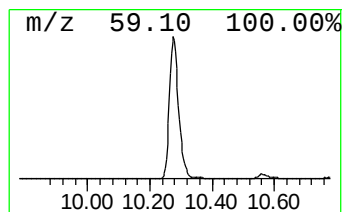
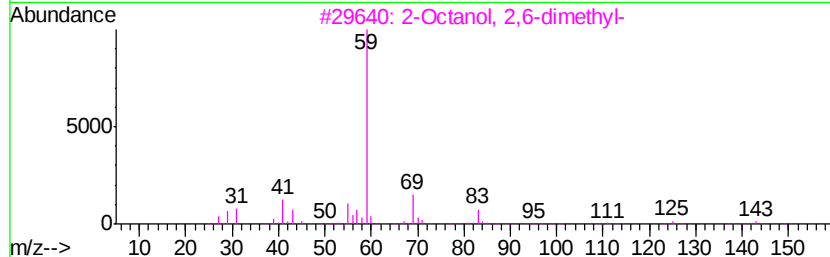
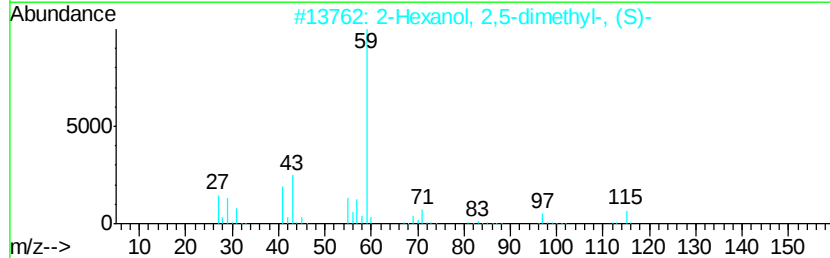
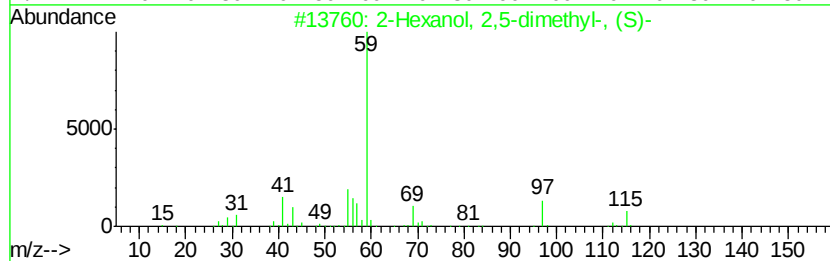
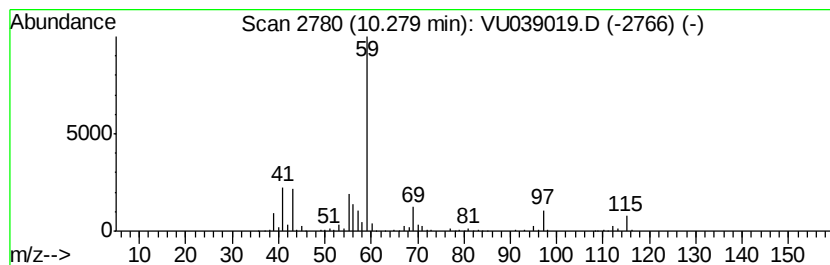
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.28	3.49 ug/L	626880	Chlorobenzene-d5	9.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90
2			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	56
3			2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4			2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	45
5			2-Hydroxy-2,4-dimethyl-3-pentanone	130	C7H14O2	003212-67-7	45



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062220\
Data File : VU039019.D
Acq On : 22 Jun 2020 21:11
Operator : SY/MD
Sample : L3061-08
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

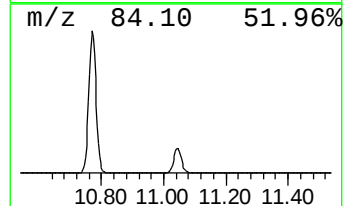
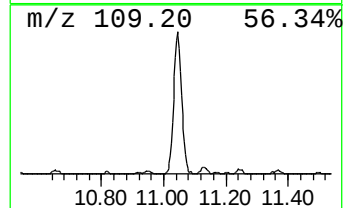
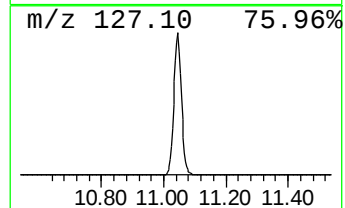
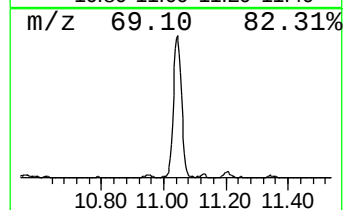
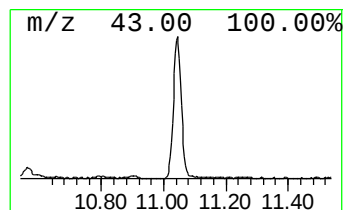
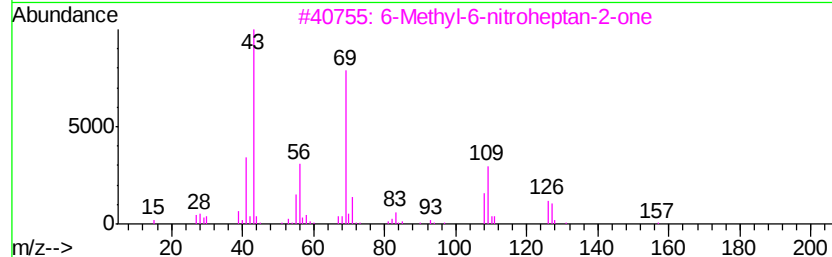
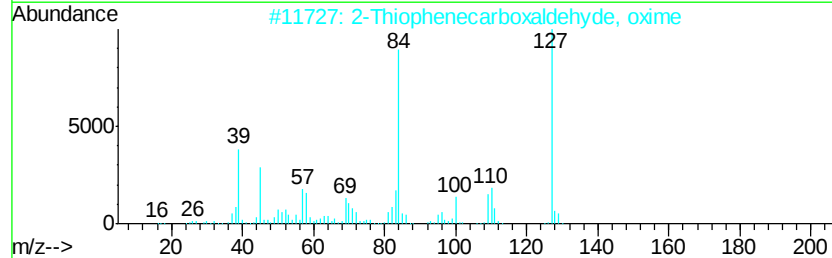
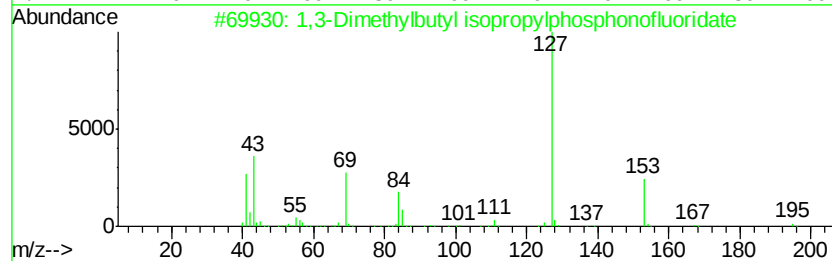
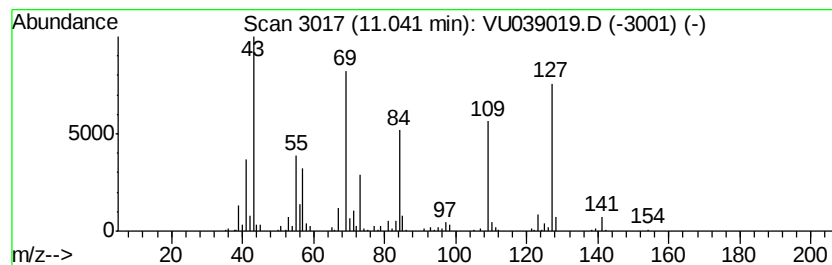
Instrument :
MSVOA_U
ClientSampleId :
BFXJ5

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 12 1,3-Dimethylbutyl isopropyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.		
11.04	1.92 ug/L	305930	1,4-Dichlorobenzene-d4	11.83		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethylbutyl isopropylphosp...	210	C9H20F02P	1000298-25-6	53	
2	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35	
3	6-Methyl-6-nitroheptan-2-one	173	C8H15NO3	142963-25-5	32	
4	Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	27	
5	Cyclohexanemethanol, .alpha.-met...	182	C12H22O	085312-76-1	27	



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062220\
 Data File : VU039019.D
 Acq On : 22 Jun 2020 21:11
 Operator : SY/MD
 Sample : L3061-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXJ5

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062220WMA.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	1.49	3.1	ug/L	405028	1	6.28	645833	5.0
Isopropyl Alcohol	2.82	0.6	ug/L	82213	1	6.28	645833	5.0
2-Propanol, 2-met...	3.23	4.6	ug/L	589968	1	6.28	645833	5.0
Diisopropyl ether	4.03	1.4	ug/L	182247	1	6.28	645833	5.0
1,3-Dioxolane	4.85	1.3	ug/L	162637	1	6.28	645833	5.0
2(1H)-Pyrimidinon...	6.94	14.3	ug/L	1850220	1	6.28	645833	5.0
(DEL) Alkane: Str...	7.36	0.8	ug/L	104564	1	6.28	645833	5.0
(DEL) Alkane: Str...	7.54	1.4	ug/L	173982	1	6.28	645833	5.0
Furan, tetrahydro...	7.74	4.9	ug/L	636293	1	6.28	645833	5.0
2-Hexanol, 2,5-di...	10.28	3.5	ug/L	626880	2	9.44	898001	5.0
1,3-Dimethylbutyl...	11.04	1.9	ug/L	305930	3	11.83	797800	5.0