

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
 Data File : VV017022.D
 Acq On : 22 Jun 2020 17:22
 Operator : SY/MD
 Sample : L3067-01
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXF8

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_V\METHOD\SOMVTR061720WMA.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	2.132	312	324	338	rBV	1412460	2157940	2.42%	1.456%
2	3.213	640	660	680	rBV	9057378	19110872	21.47%	12.896%
3	4.647	1078	1106	1136	rBV2	32716700	89010000	100.00%	60.066%
4	6.344	1615	1634	1661	rBV	1558286	3181749	3.57%	2.147%
5	7.164	1873	1889	1909	rBV	873901	1675080	1.88%	1.130%
6	9.752	2671	2694	2708	rBV	3876411	6062127	6.81%	4.091%
7	10.508	2915	2929	2953	rVB	15231314	25818998	29.01%	17.423%
8	11.556	3242	3255	3272	rBV2	716984	1171065	1.32%	0.790%

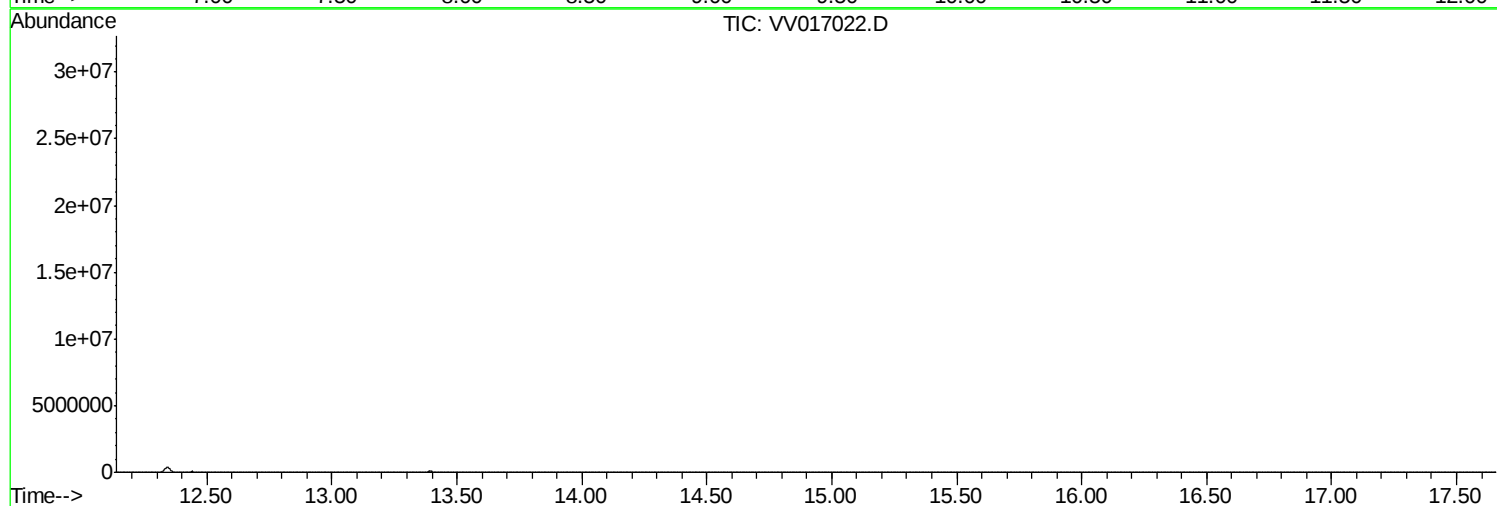
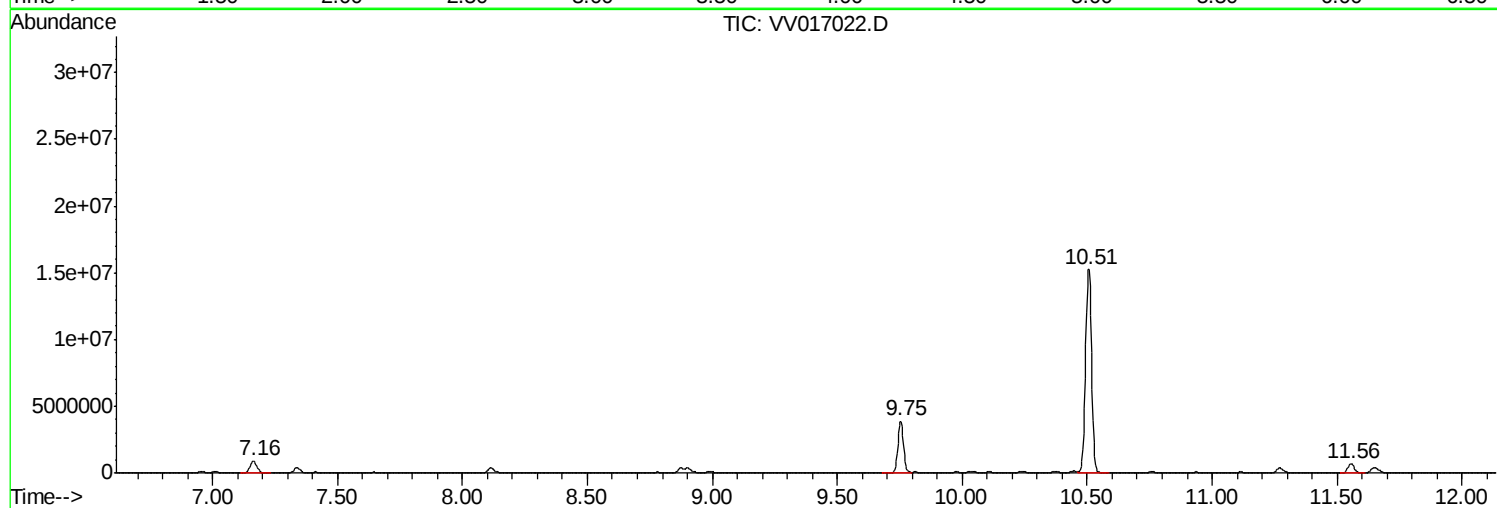
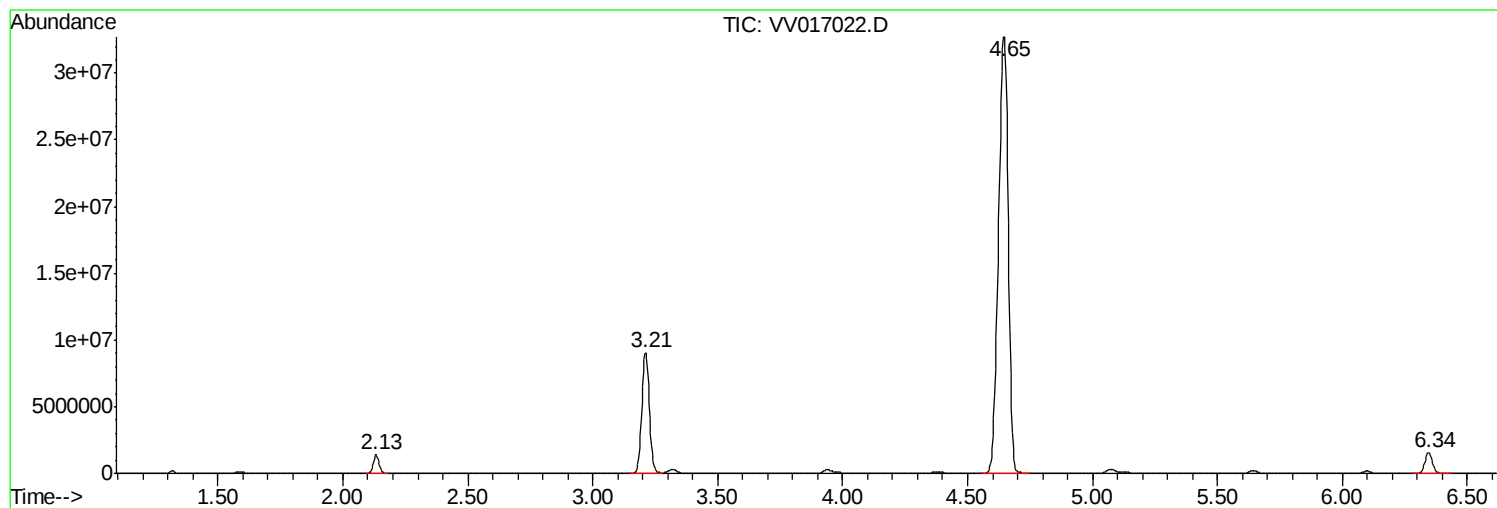
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Quant Title : TRACE VOA SOM01.0

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



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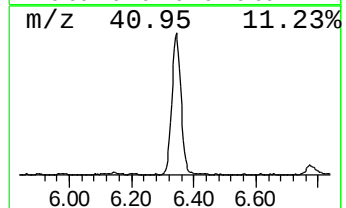
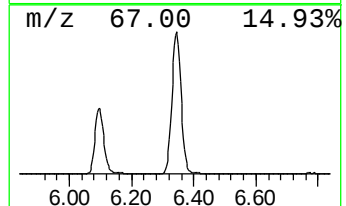
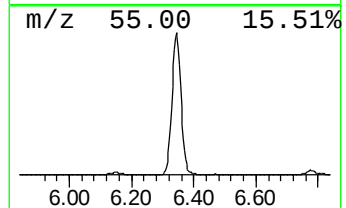
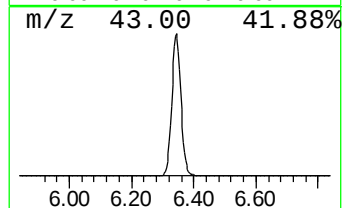
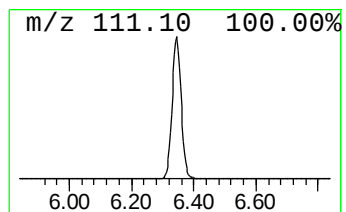
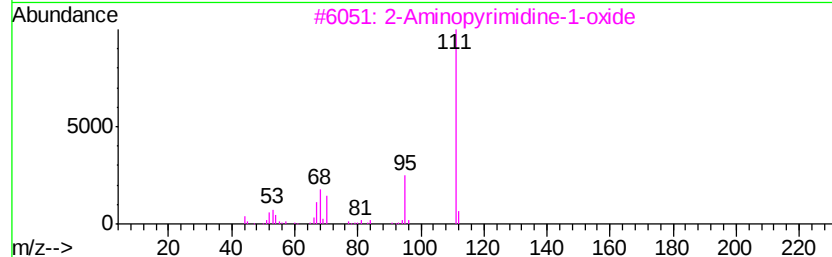
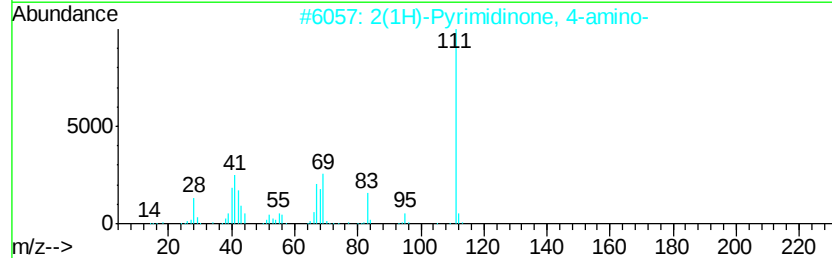
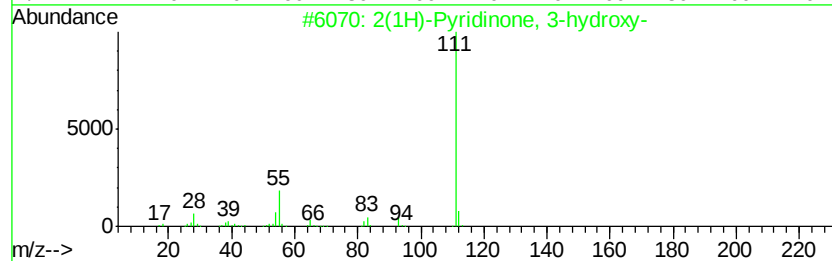
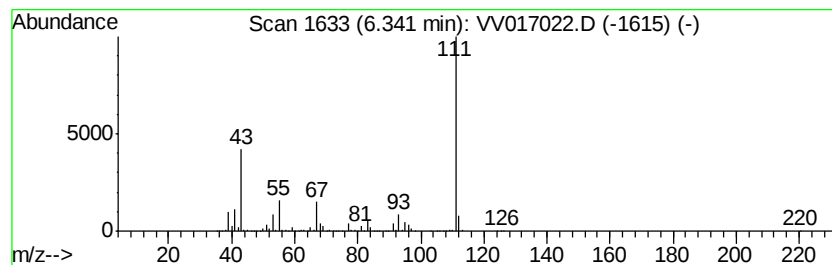
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 2(1H)-Pyridinone, 3-hydroxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	5.00 ug/L	3181750	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(1H)-Pyridinone, 3-hydroxy-	111	C5H5NO2	016867-04-2	64
2			2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
3			2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	50
4			2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39
5			Bruceantin	548	C28H36O11	041451-75-6	39



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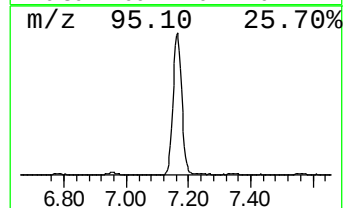
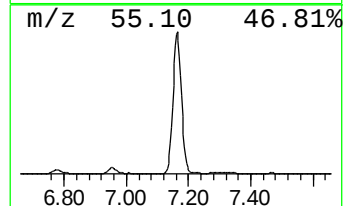
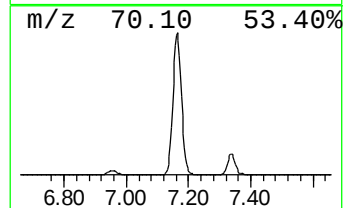
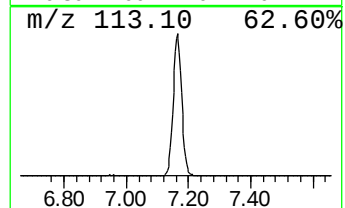
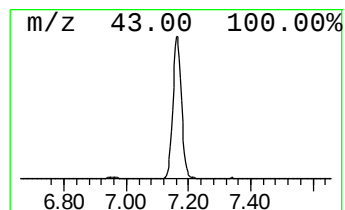
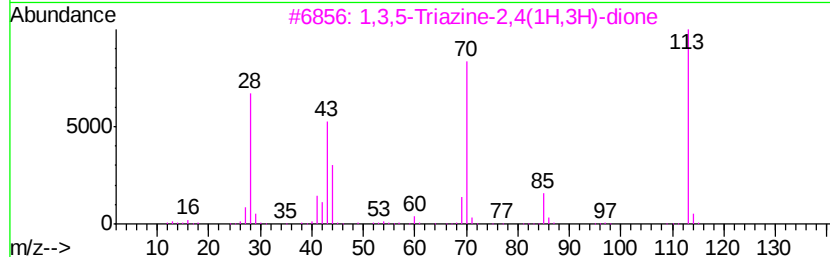
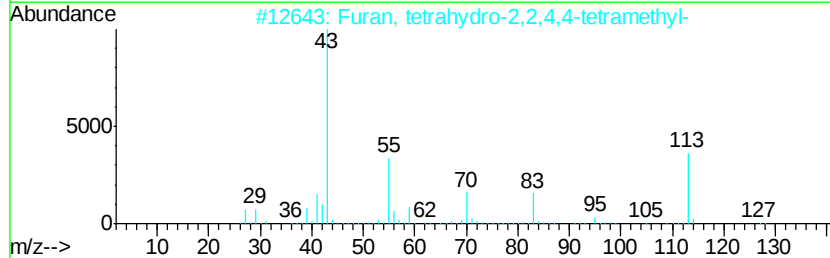
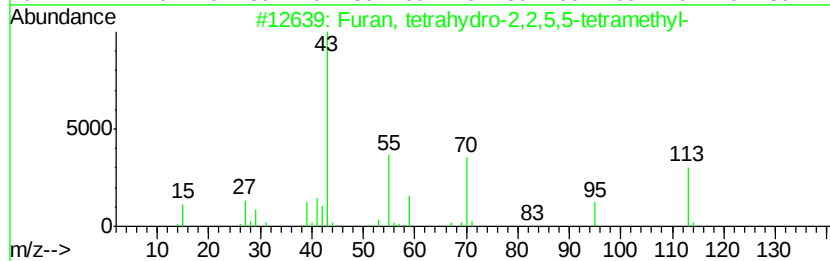
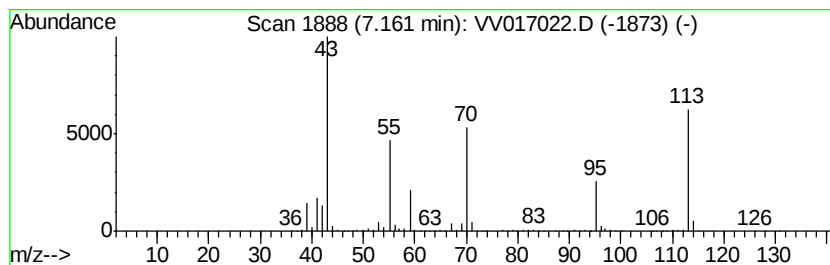
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Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.16	2.63 ug/L	1675080	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2		Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
3		1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	47
4		Propanone-1, 3-(4-methylpiperazi...	308	C20H24N2O	053756-76-6	43
5		Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	42



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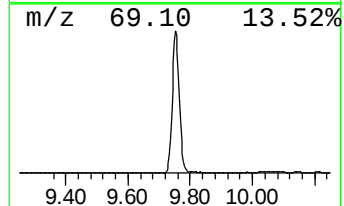
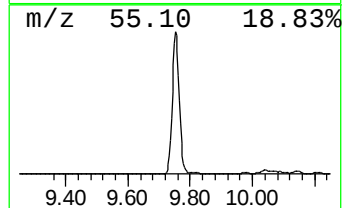
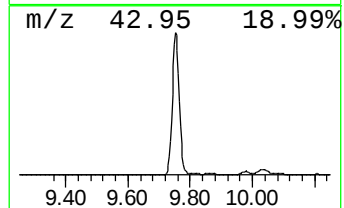
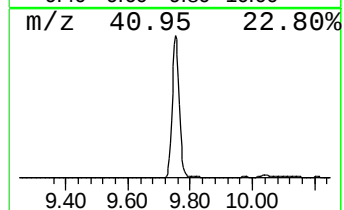
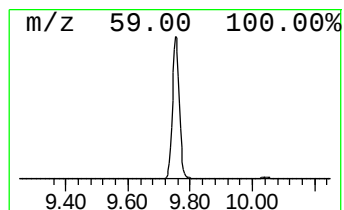
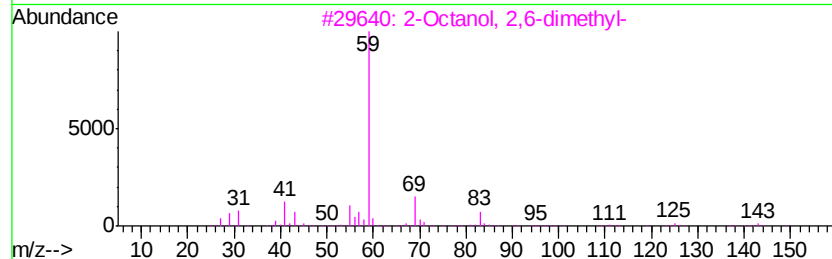
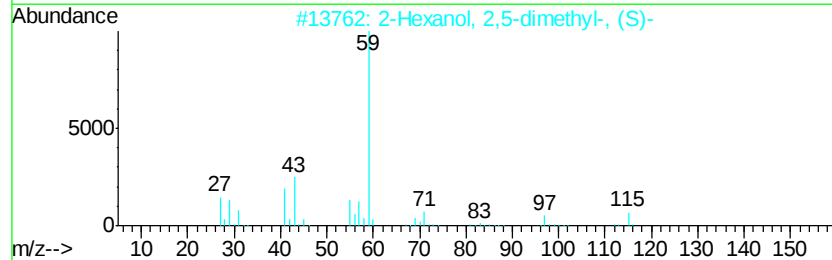
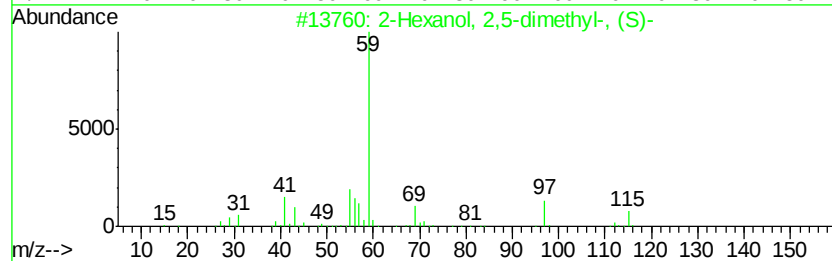
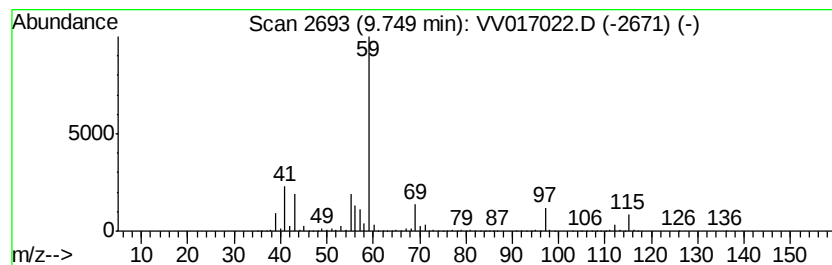
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.75	5.00 ug/L	6062130	Chlorobenzene-d5	8.87

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	78
3		2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	64
4		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	42
5		Cyclohexane, (ethoxymethoxy)-	158	C9H18O2	054699-29-5	38



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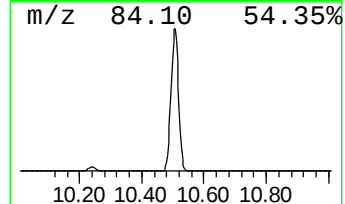
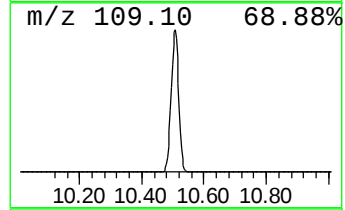
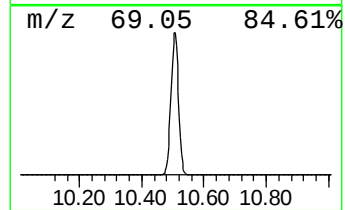
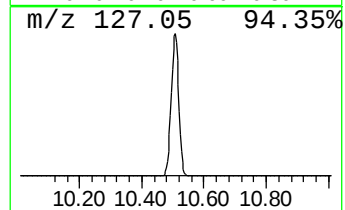
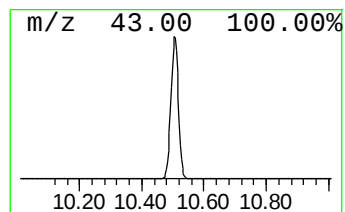
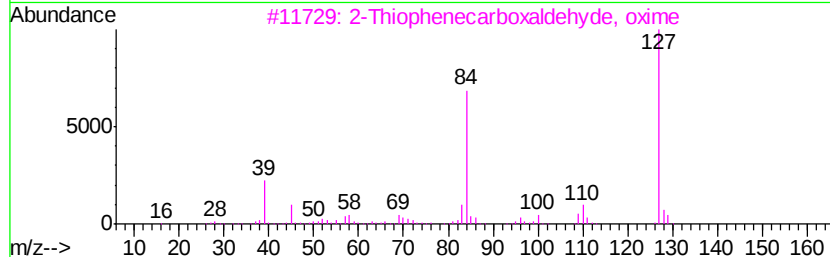
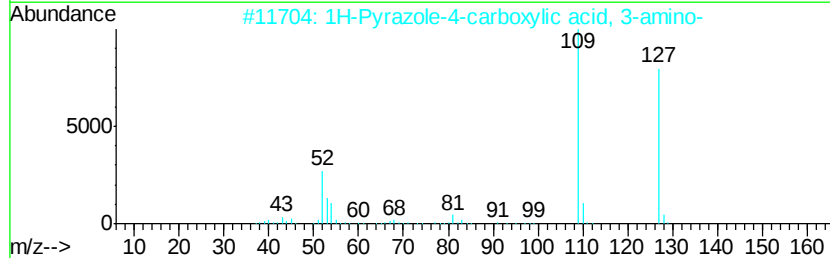
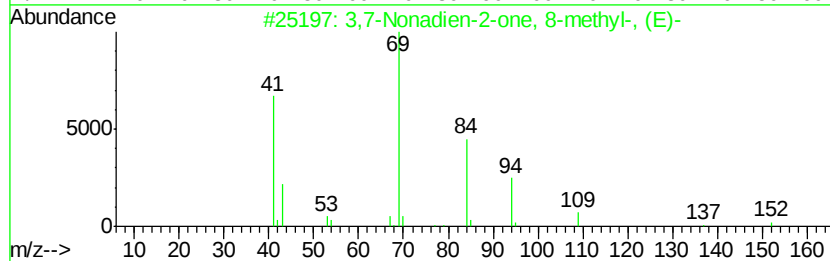
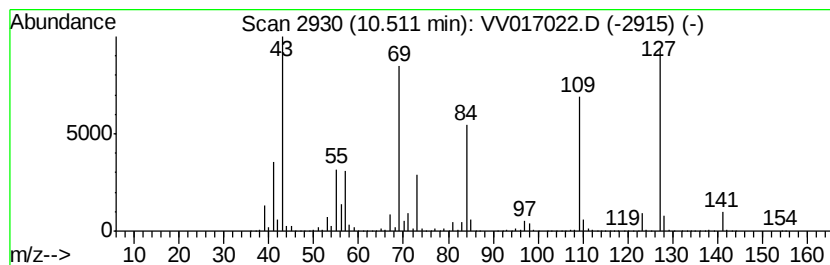
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.51	110.24 ug/L	25819000	1,4-Dichlorobenzene-d4	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7-Nonadien-2-one, 8-methyl-, (E)-	152	C10H16O		035408-14-1	35
2	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2		041680-34-6	35
3	2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS		029683-84-9	35
4	Ethanone, 1-cyclopropyl-	84	C5H8O		000765-43-5	27
5	2-Pentene, 4-methyl-, (Z)-	84	C6H12		000691-38-3	27



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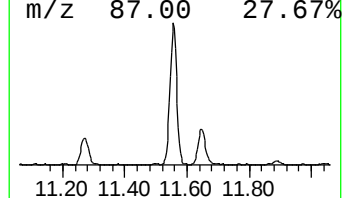
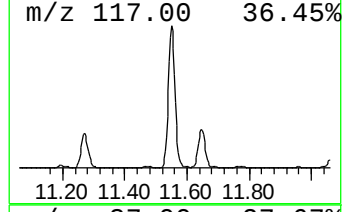
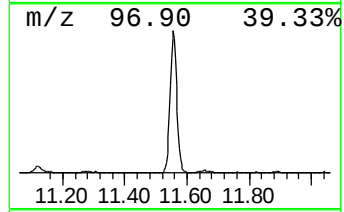
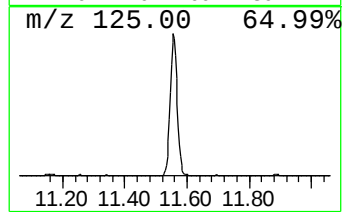
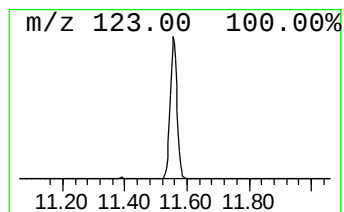
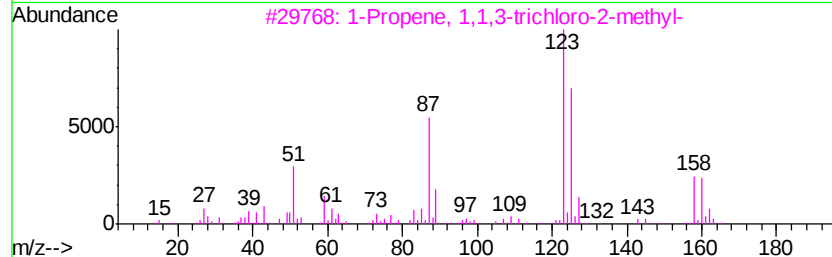
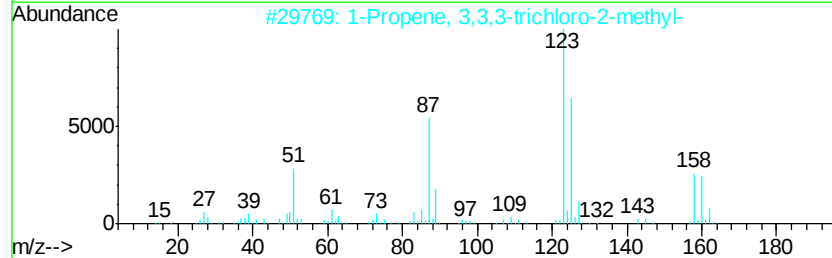
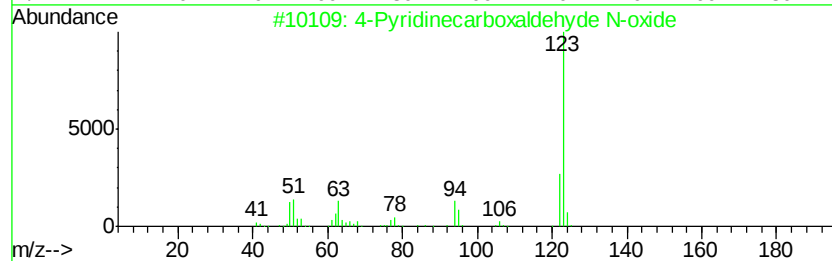
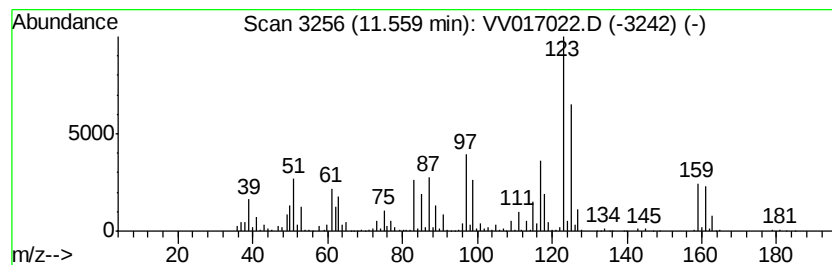
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	5.00 ug/L	1171070	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Pyridinecarboxaldehyde N-oxide	123	C6H5NO2	007216-42-4	22
2		1-Propene, 3,3,3-trichloro-2-met...	158	C4H5Cl3	004749-27-3	12
3		1-Propene, 1,1,3-trichloro-2-met...	158	C4H5Cl3	031702-33-7	12
4		Methyl 3,3-dichloropropenoate	154	C4H4Cl2O2	002257-46-7	12
5		Benzoyl chloride, 2-fluoro-	158	C7H4ClFO	000393-52-2	12



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2(1H)-Pyridinone,...	6.34	5.0	ug/L	3181750	1	5.64	3181750	5.0
Furan, tetrahydro...	7.16	2.6	ug/L	1675080	1	5.64	3181750	5.0
2-Hexanol, 2,5-di...	9.75	5.0	ug/L	6062130	2	8.87	6062130	5.0
unknown-01	10.51	110.2	ug/L	25819000	3	11.27	1171070	5.0
unknown-02	11.56	5.0	ug/L	1171070	3	11.27	1171070	5.0