LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062320\
Data File : VV017039.D
Acq On : 23 Jun 2020 00:09
Operator : SY/MD
Sample : L3067-11
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFXG8

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	1.116	4	8	17	rVB3	11438	13748	2.16%	0.226%
2	1.315	63	70	81	rVB	85352	85836	13.47%	1.408%
3	1.460	97	115	118	rBV2	23508	65362	10.26%	1.072%
4	1.579	145	152	162	rVB	66338	75813	11.90%	1.244%
5	2.122	312	321	338	rBV	134816	199223	31.27%	3.269%
6	3.212	651	660	670	rVB4	5006	9914	1.56%	0.163%
7	3.929	868	883	914	rBV	72223	261332	41.02%	4.288%
8	4.376	1007	1022	1044	rBV2	109946	276618	43.42%	4.539%
9	4.634	1085	1102	1116	rBV4	18465	50557	7.94%	0.830%
10	5.071	1221	1238	1261	rBV2	260859	637111	100.00%	10.454%
11	5.640	1398	1415	1439	rBV	214690	438179	68.78%	7.190%
12	6.093	1540	1556	1574	rBV	144914	297437	46.69%	4.880%
13	6.344	1616	1634	1649	rBV3	25326	57405	9.01%	0.942%
14	6.955	1816	1824	1831	rBV5	9957	15882	2.49%	0.261%
15	7.010	1831	1841	1858	rVB	72345	130972	20.56%	2.149%
16	7.158	1878	1887	1901	rBV4	12323	24603	3.86%	0.404%
17	7.338	1931	1943	1962	rBV	321856	557645	87.53%	9.150%
18	7.643	2029	2038	2049	rBV	44247	75254	11.81%	1.235%
19	8.113	2171	2184	2210	rBV	282492	538525	84.53%	8.836%
20	8.871	2407	2420	2438	rBV	328083	539990	84.76%	8.860%
21	9.756	2682	2695	2707	rBV2	35400	62393	9.79%	1.024%
22	10.238	2834	2845	2857	rBV	104402	160658	25.22%	2.636%
23	10.502	2915	2927	2942	rBV	257494	427170	67.05%	7.009%
24	10.720	2989	2995	3006	rVB9	4066	6953	1.09%	0.114%
25	11.270	3154	3166	3189	rVV	351104	544988	85.54%	8.942%
26	11.646	3270	3283	3305	rBV	327460	522516	82.01%	8.574%
27	16.337	4733	4742	4752	rVB6	11353	18422	2.89%	0.302%

Sum of corrected areas: 6094506

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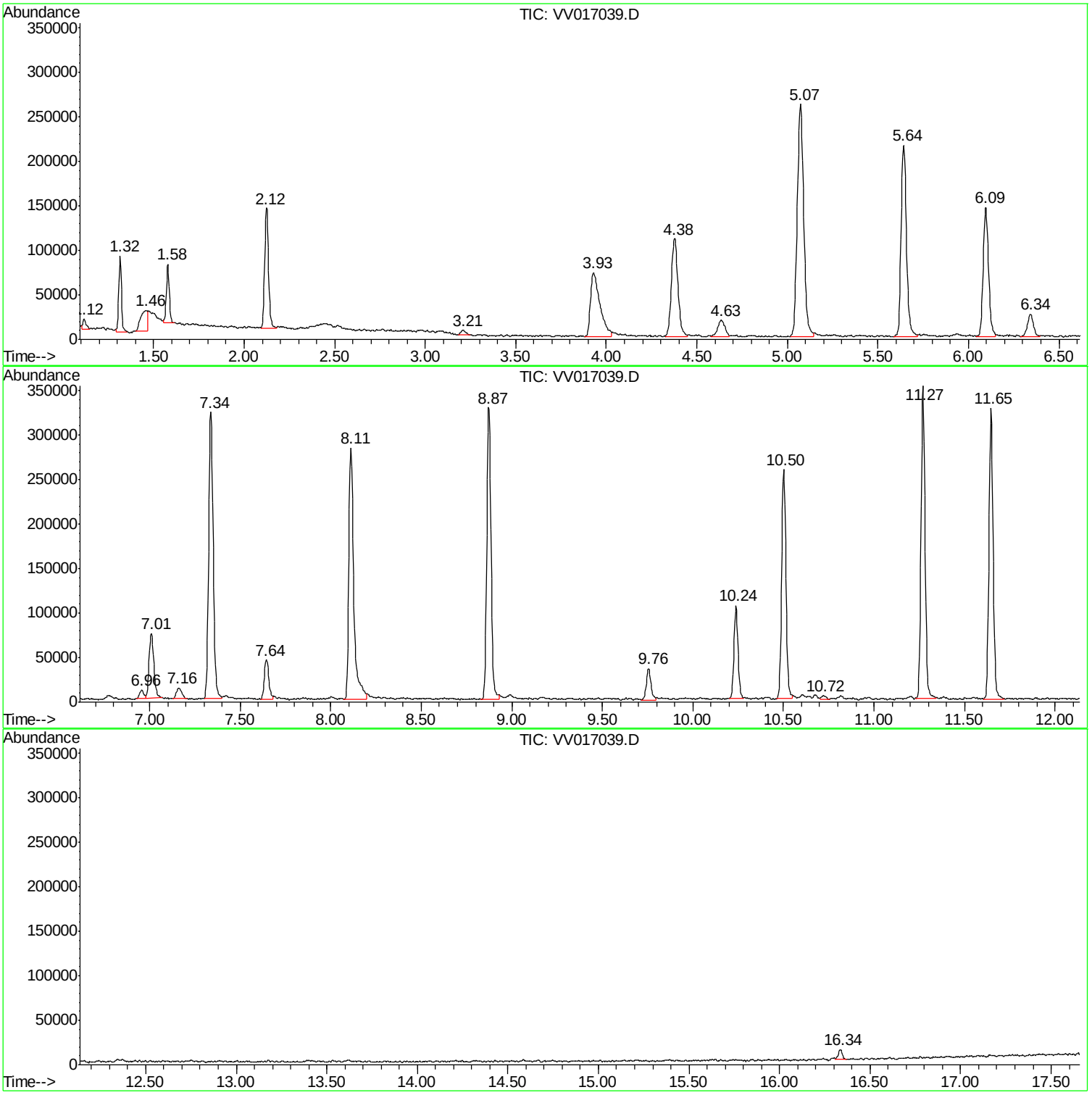
Instrument : MSVOA_V
ClientSampleId : BFXG8

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

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



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Quant Title : TRACE VOA SOM01.0

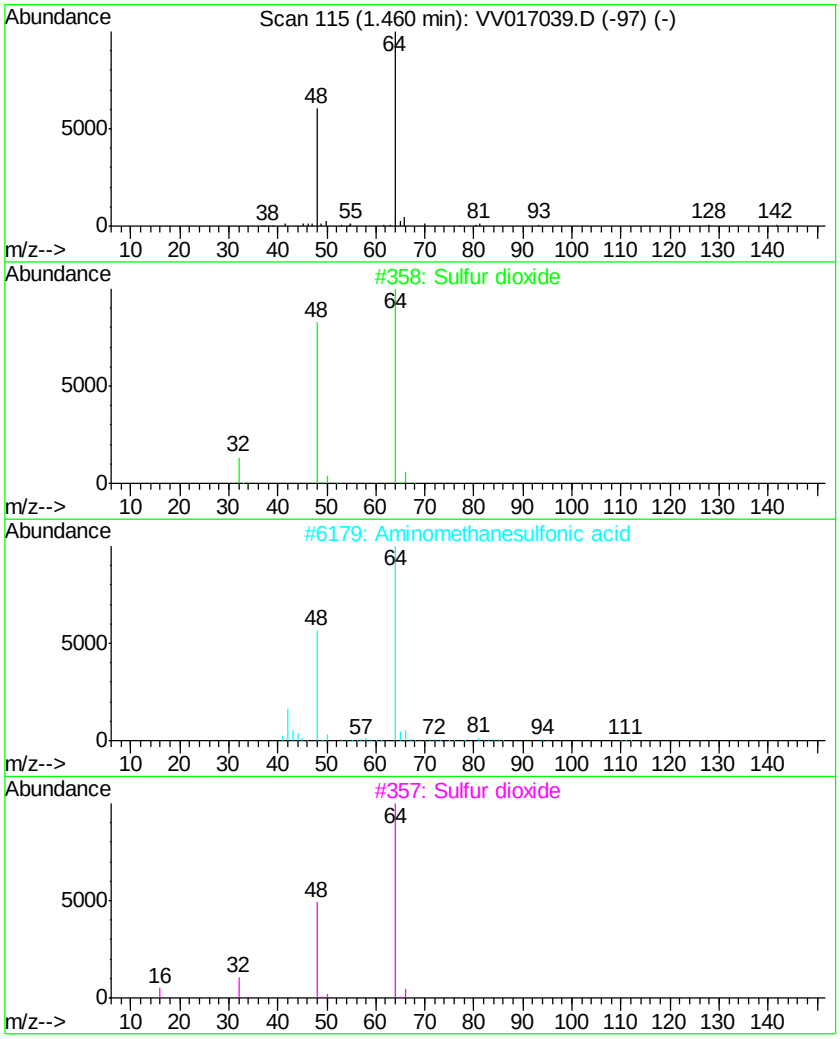
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

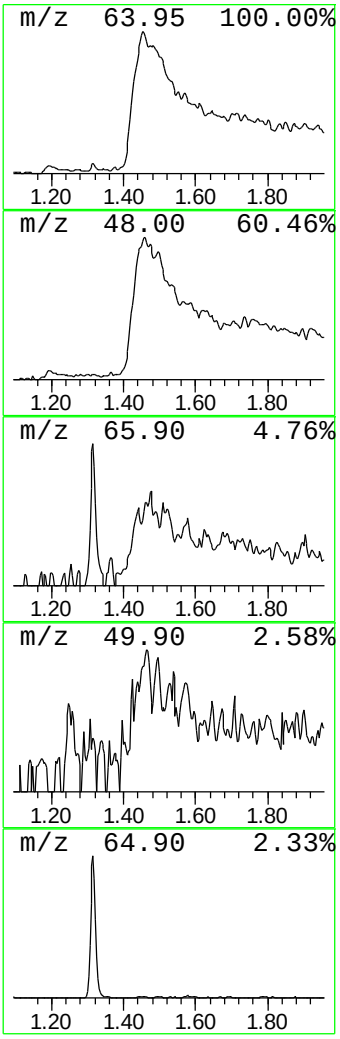
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.46	0.75 ug/L	65362	1,4-Difluorobenzene	5.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	74
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	Sulfur dioxide	64	O2S	007446-09-5	74
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV062320\
Data File : VV017039.D
Acq On : 23 Jun 2020 00:09
Operator : SY/MD
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Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFXG8

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

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

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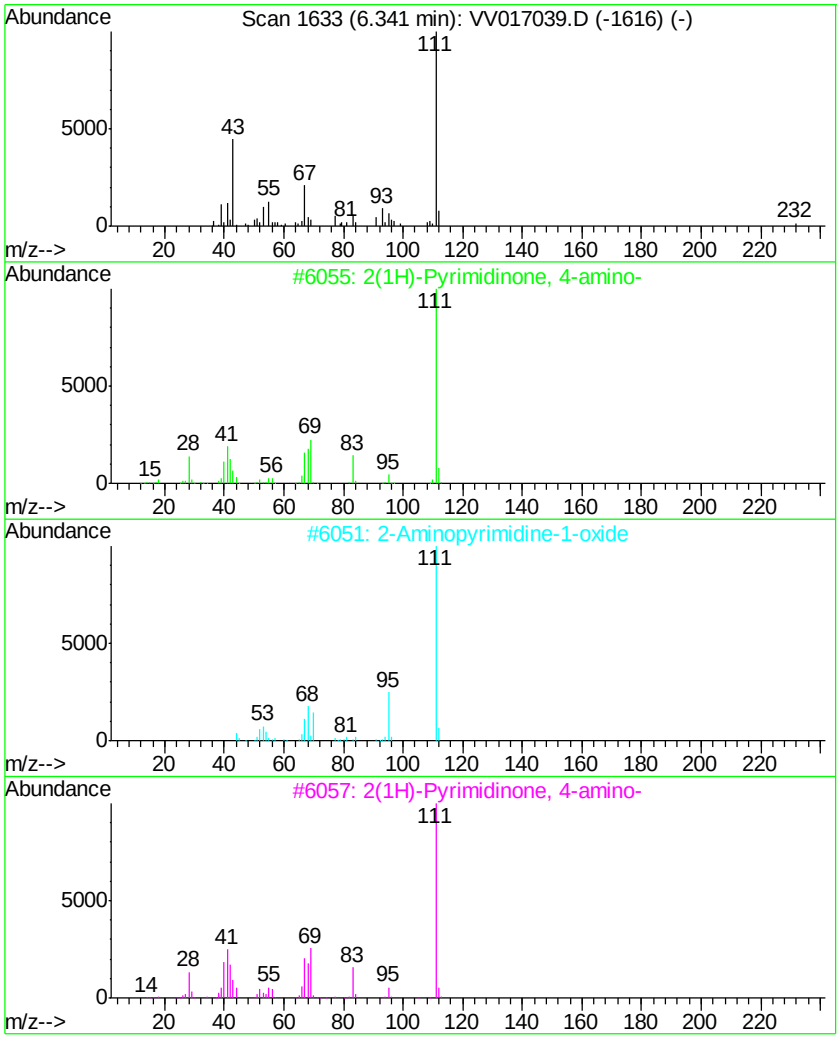
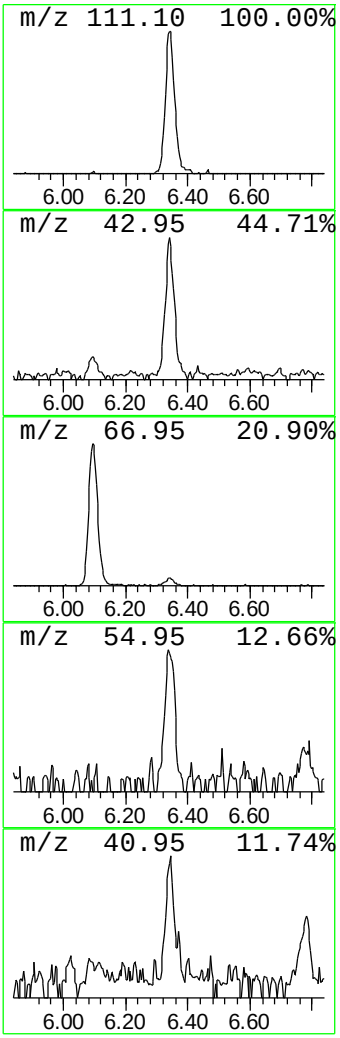
Peak Number 2 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	0.66 ug/L	57405	1,4-Difluorobenzene	5.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	72
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	64
3	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64
4	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	56
5	Montanol	352	C21H36O4	1000145-58-3	53





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Operator : SY/MD
Sample : L3067-11
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : BFXG8

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

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

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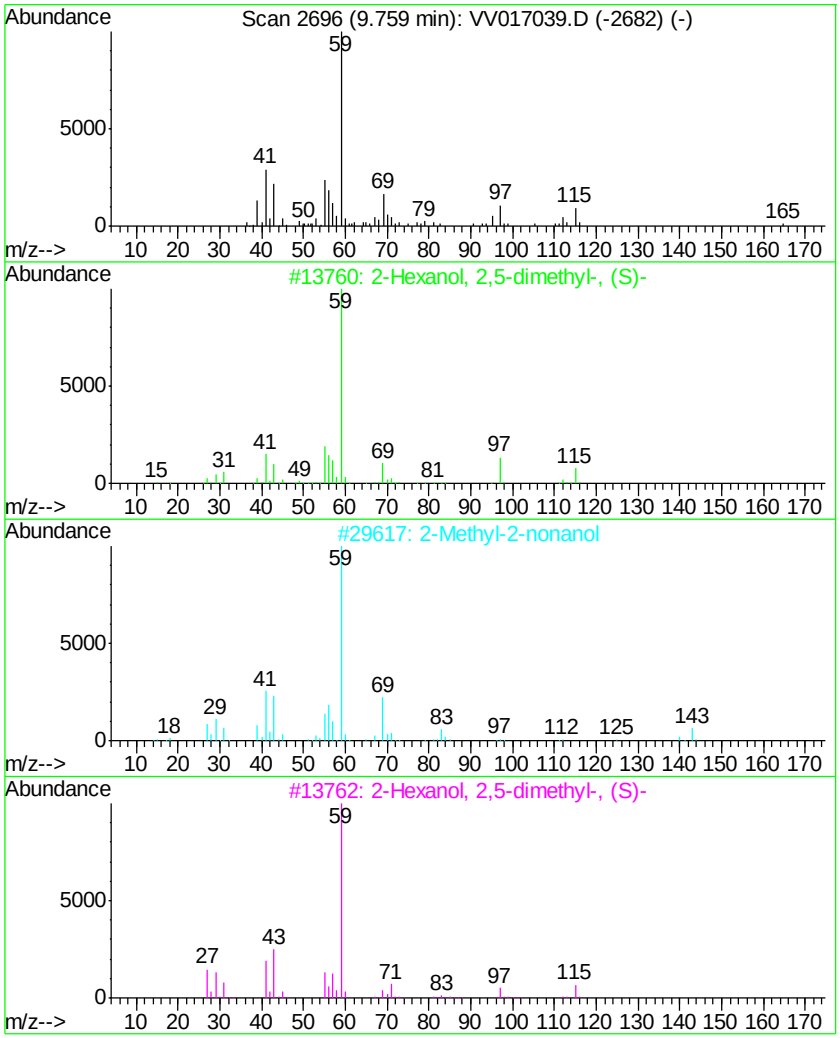
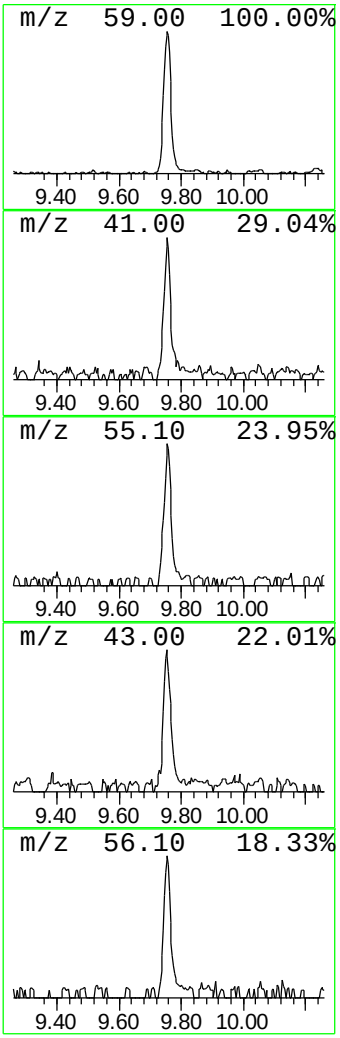
Peak Number 4 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.76	0.58 ug/L	62393	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	83
2	2-Methyl-2-nonanol	158	C10H22O	010297-57-1	64
3	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	59
4	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	58
5	Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	47





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Instrument : MSVOA_V
ClientSampleId : BFXG8

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

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

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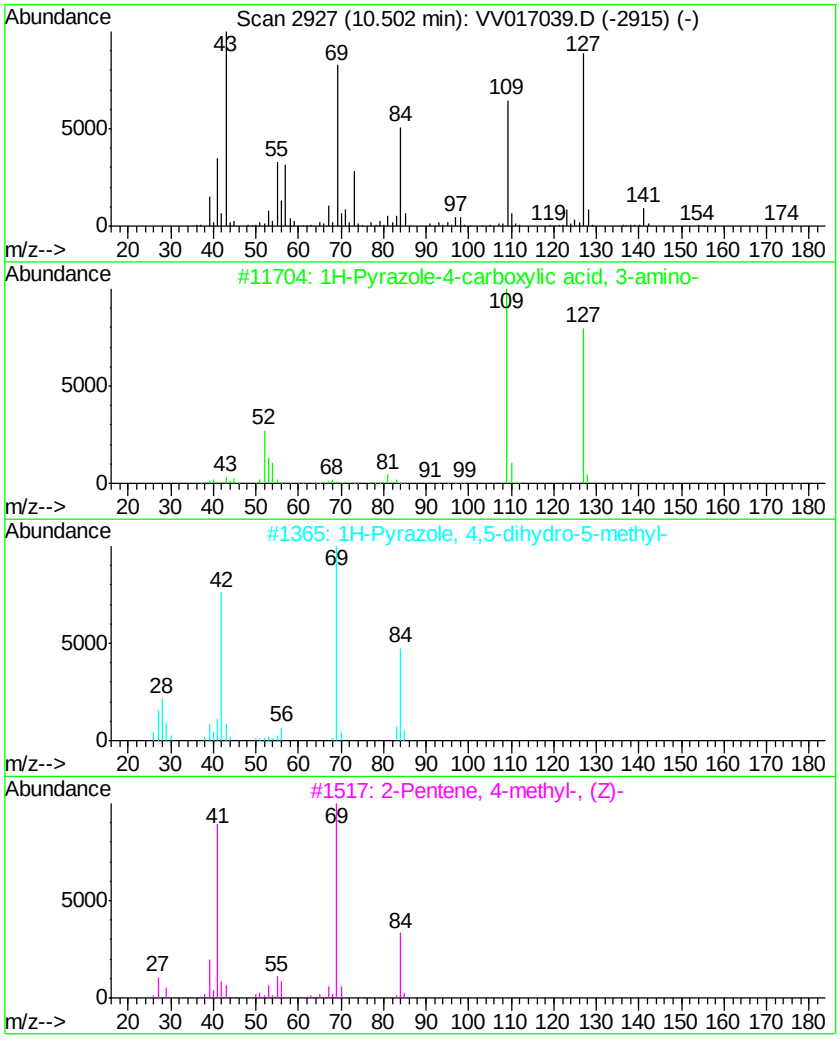
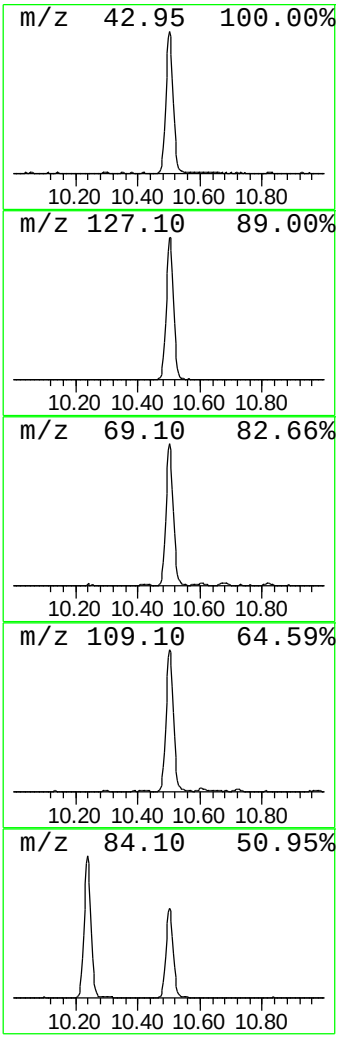
Peak Number 5 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	3.92 ug/L	427170	1,4-Dichlorobenzene-d4	11.27

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
2	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	30
3	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27
4	4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	22
5	2-Hydroxy-4-hydroxylaminopyrimidine	127	C4H5N3O2	020555-88-8	22





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.46	0.8	ug/L	65362	1	5.64	438179	5.0
2(1H)-Pyrimidinon...	6.34	0.7	ug/L	57405	1	5.64	438179	5.0
2-Hexanol, 2,5-di...	9.76	0.6	ug/L	62393	2	8.87	539990	5.0
unknown-01	10.50	3.9	ug/L	427170	3	11.27	544988	5.0