LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081920\
Data File : VX017991.D
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 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_X\METHOD\82X081920W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	27	29	36	rVV	878071	1274231	6.79%	2.065%
2	1.325	36	39	52	rVB	98170	356783	1.90%	0.578%
3	1.569	75	79	93	rBV	5623872	6335914	33.78%	10.268%
4	2.251	186	191	201	rVB2	120715	197109	1.05%	0.319%
5	2.422	213	219	223	rBV	1136569	1922524	10.25%	3.116%
6	2.465	223	226	233	rVB	652885	984290	5.25%	1.595%
7	2.550	233	240	252	rBV	7689630	12806650	68.27%	20.754%
8	5.470	704	719	732	rBV2	293500	868812	4.63%	1.408%
9	5.629	732	745	759	rVV	485620	1368705	7.30%	2.218%
10	6.031	798	811	819	rBV	306661	771984	4.12%	1.251%
11	6.117	819	825	835	rVB2	89258	233280	1.24%	0.378%
12	6.781	926	934	935	rBV3	337023	726716	3.87%	1.178%
13	6.830	936	942	974	rVB	989584	3573692	19.05%	5.791%
14	8.470	1201	1211	1233	rBV	5026580	18758783	100.00%	30.400%
15	8.695	1241	1248	1255	rBV	1556109	2393398	12.76%	3.879%
16	8.891	1275	1280	1288	rVB	158544	238744	1.27%	0.387%
17	9.976	1451	1458	1471	rBV	260813	461389	2.46%	0.748%
18	10.098	1471	1478	1483	rBV	1419211	1927833	10.28%	3.124%
19	10.341	1509	1518	1524	rBV2	149759	262531	1.40%	0.425%
20	10.805	1590	1594	1603	rVB	155756	199878	1.07%	0.324%
21	11.122	1641	1646	1653	rVB	1254346	1522425	8.12%	2.467%
22	11.707	1737	1742	1751	rBV	749400	1016614	5.42%	1.647%
23	11.792	1751	1756	1762	rVB	163742	209165	1.12%	0.339%
24	12.061	1795	1800	1807	rVB	1559110	1892155	10.09%	3.066%
25	13.816	2082	2088	2094	rBV	1150252	1403511	7.48%	2.274%

Sum of corrected areas: 61707116

LSC Report - Integrated Chromatogram

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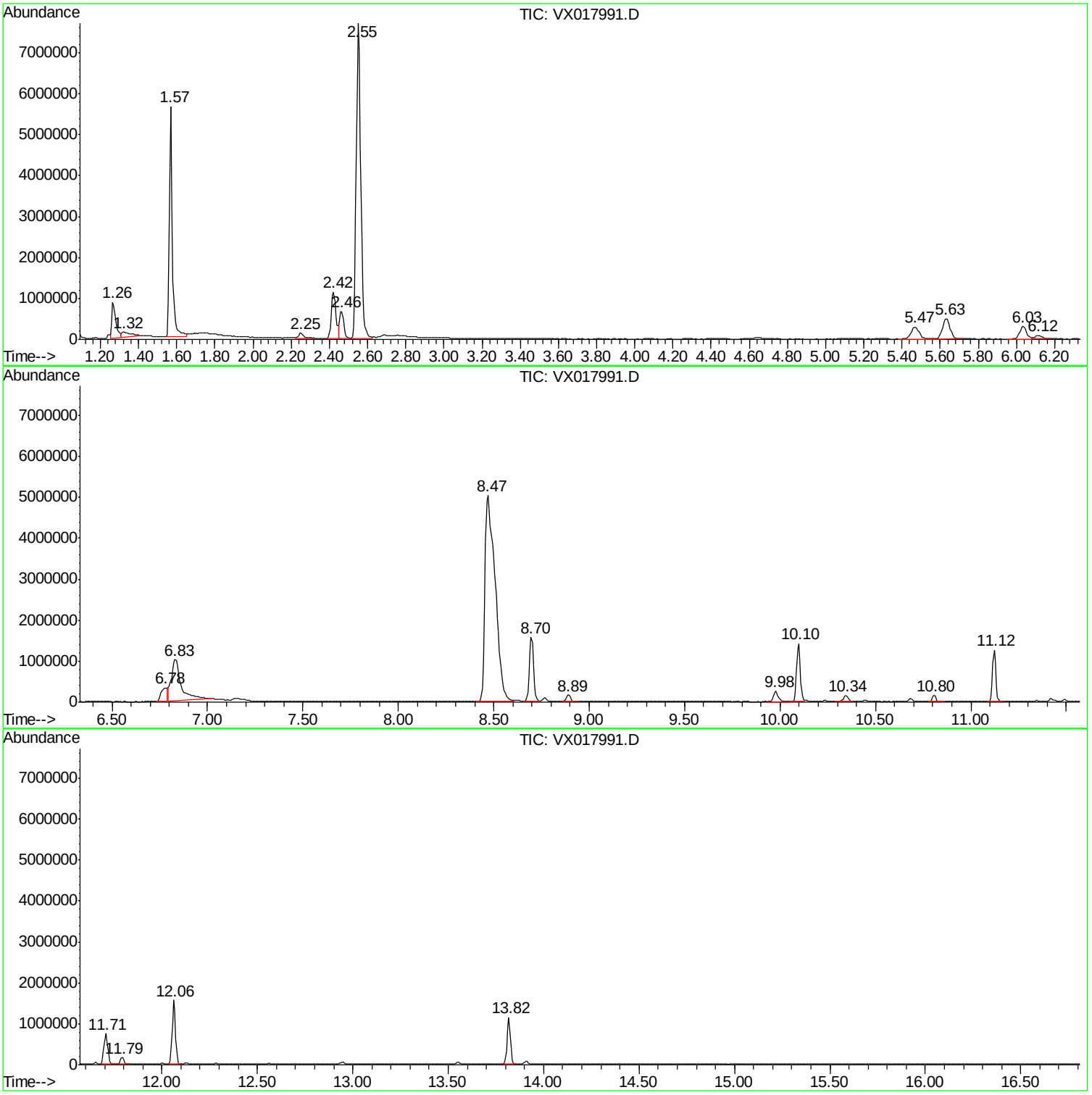
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

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



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Data File : VX017991.D
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

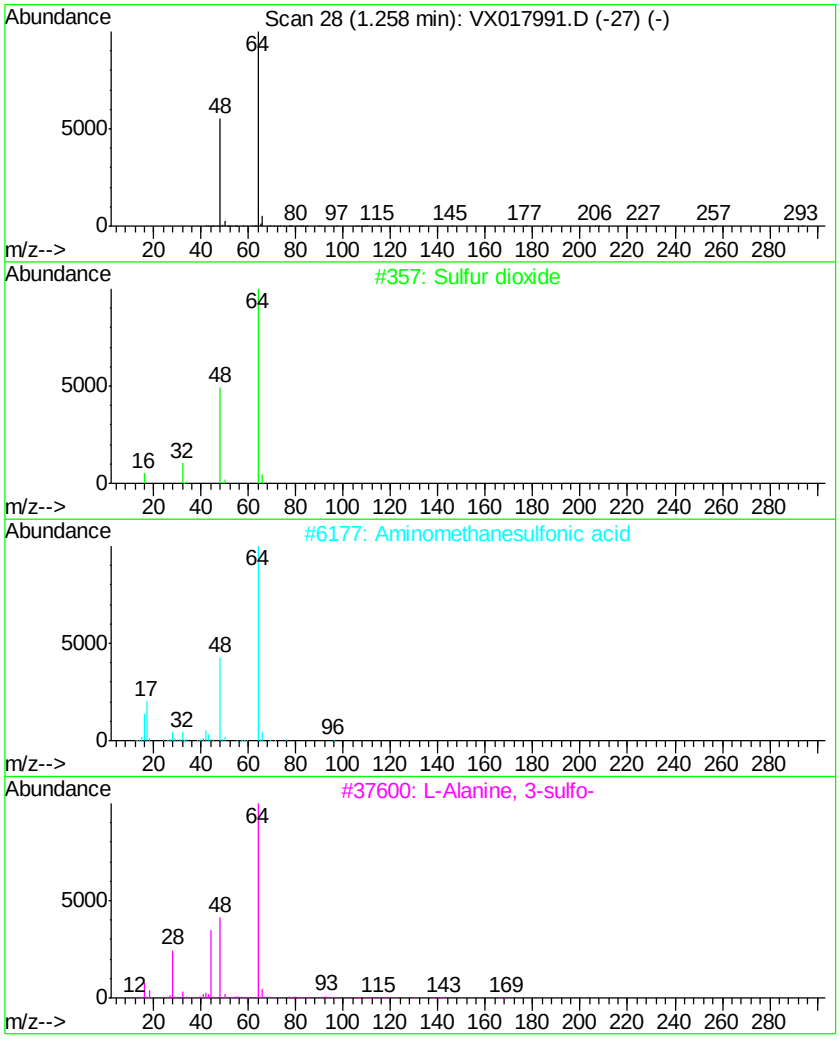
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

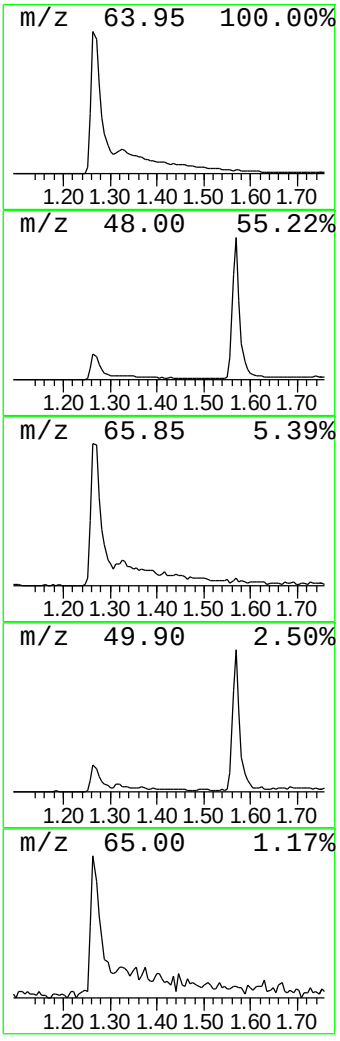
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	46.55 ug/l	1274230	Pentafluorobenzene	5.63

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	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081920\
Data File : VX017991.D
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

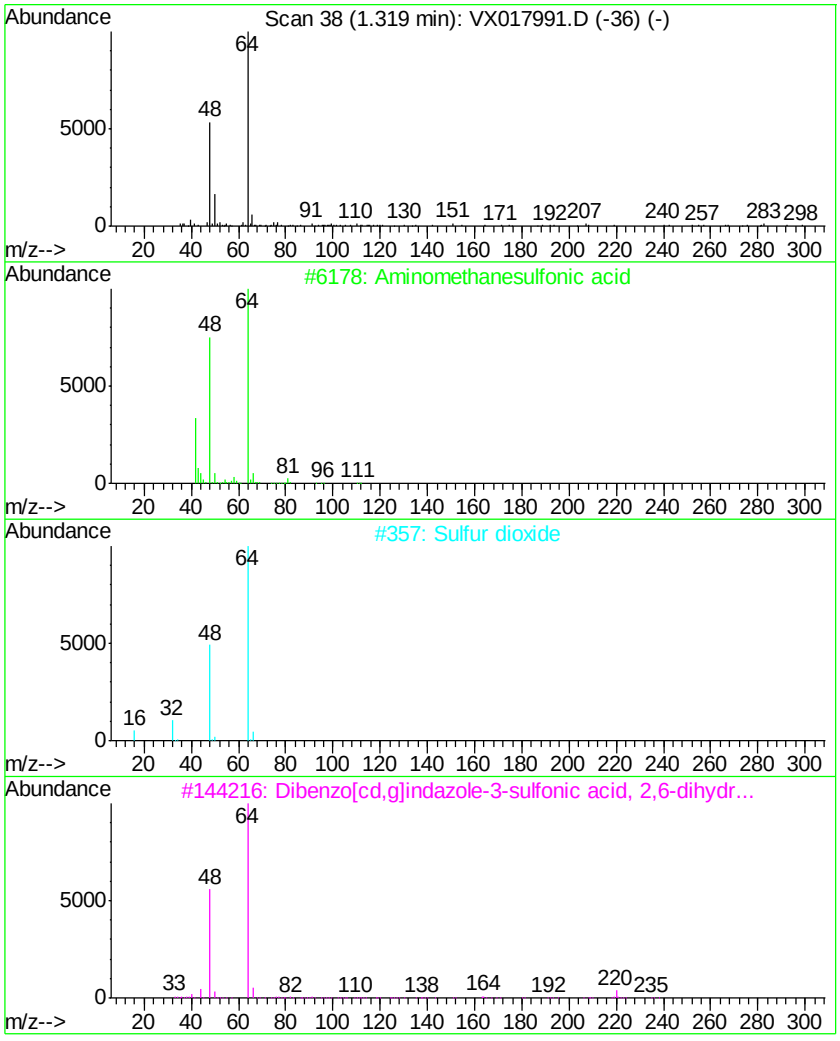
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

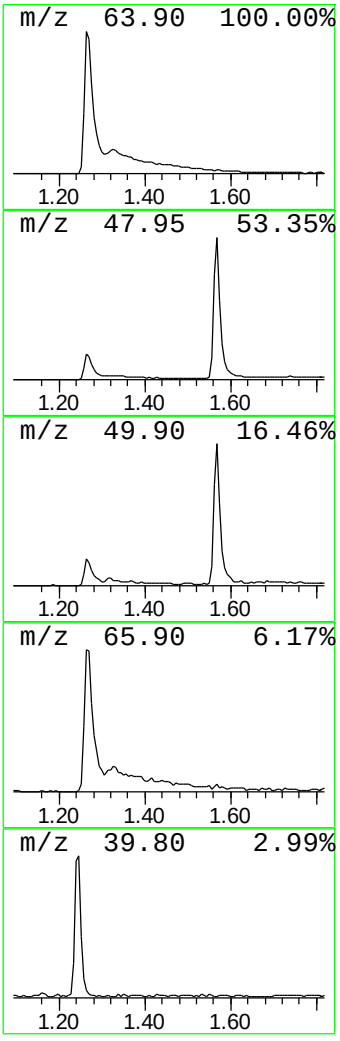
****

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	13.03 ug/l	356783	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2	Sulfur dioxide	64	O2S	007446-09-5	74
3	Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
4	Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25NO4S2	038920-47-7	64
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081920\
Data File : VX017991.D
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

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

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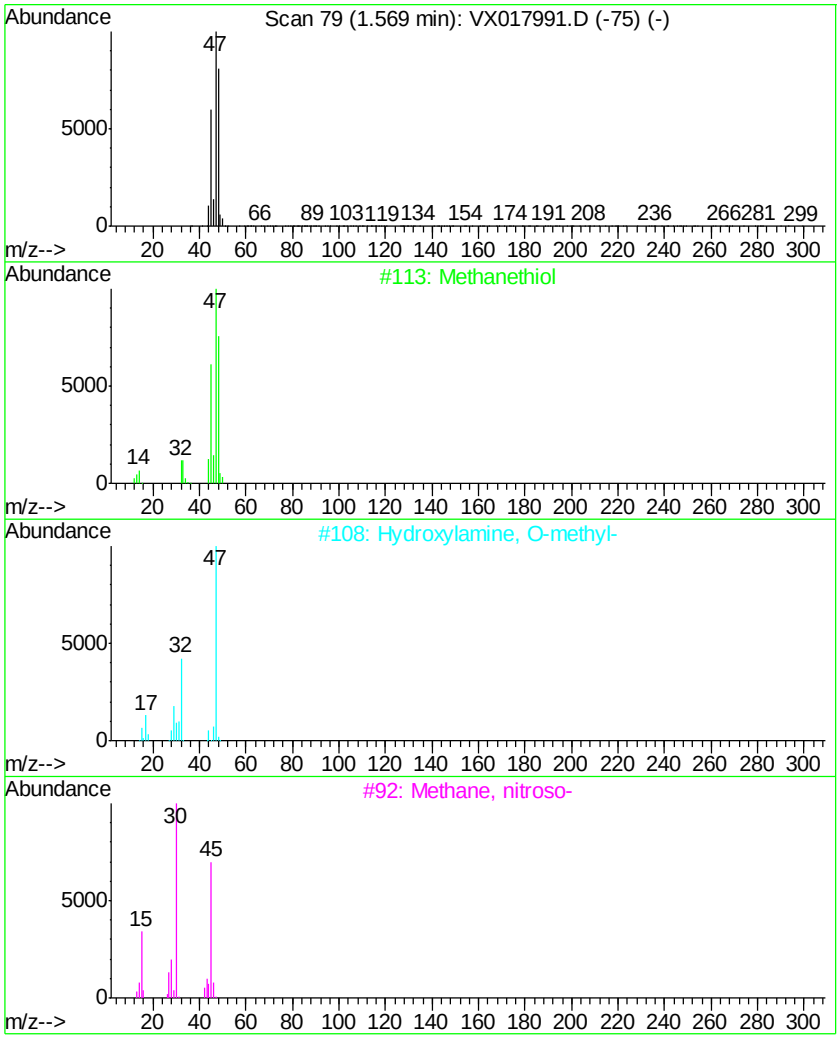
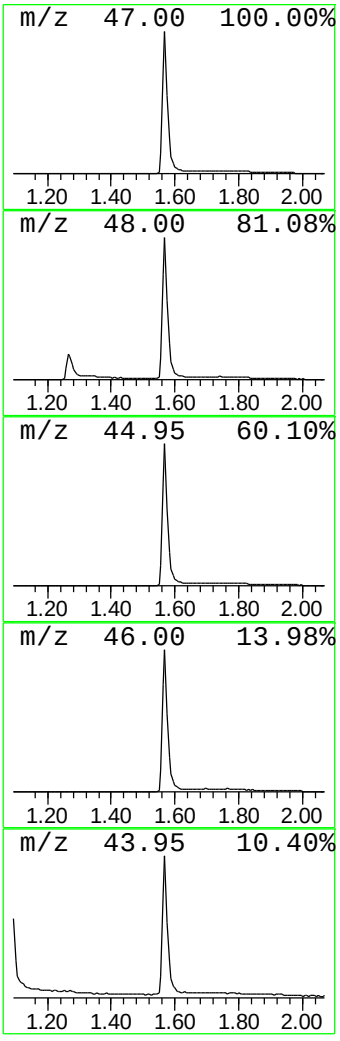
Peak Number 3 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.57	231.46 ug/l	6335910	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
3	Methane, nitroso-	45	CH3NO	000865-40-7	5
4	Ethane, fluoro-	48	C2H5F	000353-36-6	4
5	Formamide	45	CH3NO	000075-12-7	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081920\
Data File : VX017991.D
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

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

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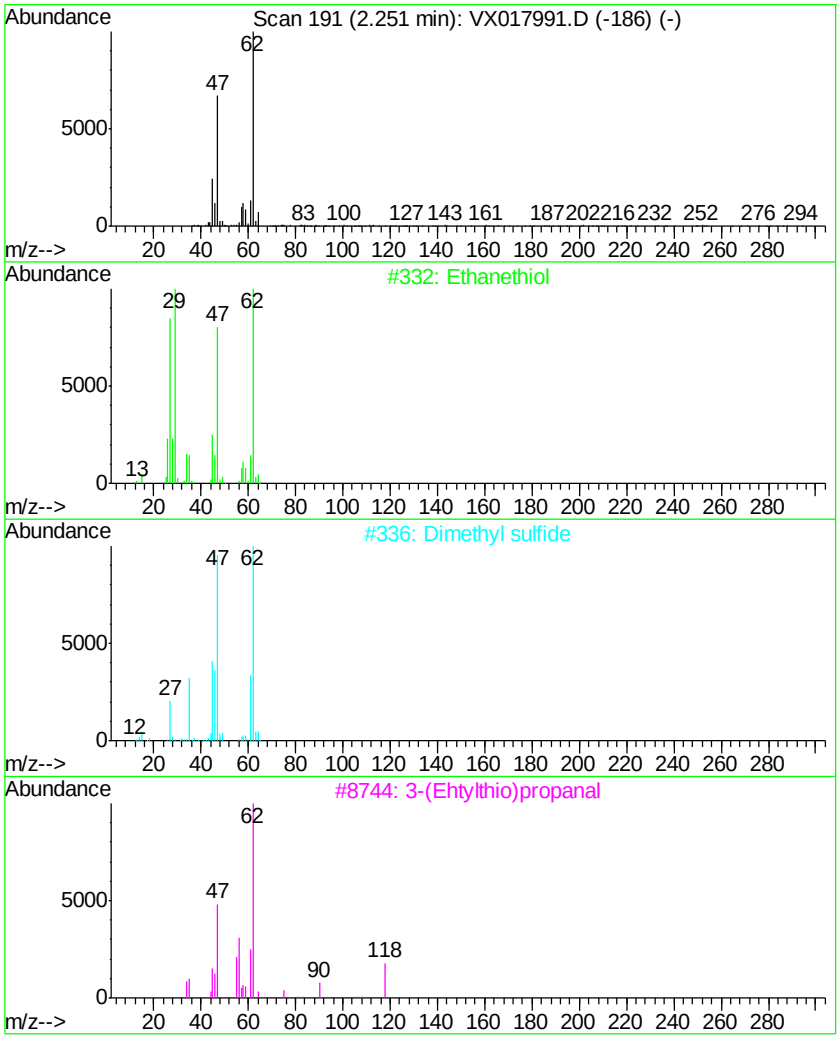
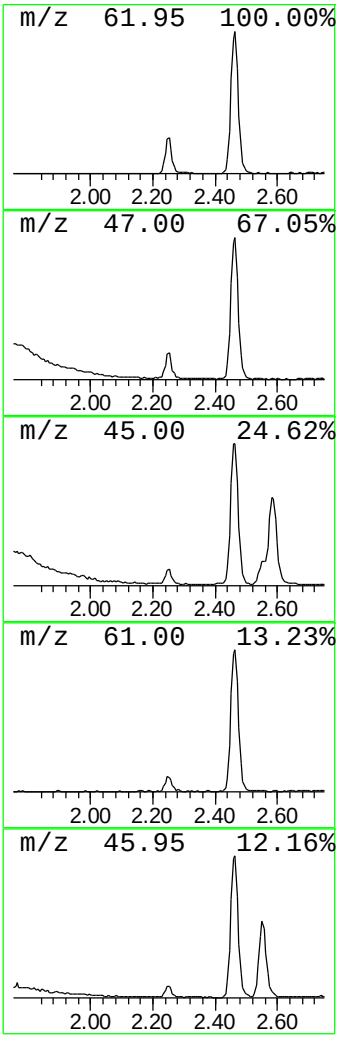
Peak Number 4 Ethanethiol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	7.20 ug/l	197109	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol	62	C2H6S	000075-08-1	91
2	Dimethyl sulfide	62	C2H6S	000075-18-3	78
3	3-(Ehtylthio)propanal	118	C5H10OS	005454-45-5	74
4	Phosphine, ethyl-	62	C2H7P	000593-68-0	72
5	Peroxide, dimethyl	62	C2H6O2	000690-02-8	50





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081920\
Data File : VX017991.D
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

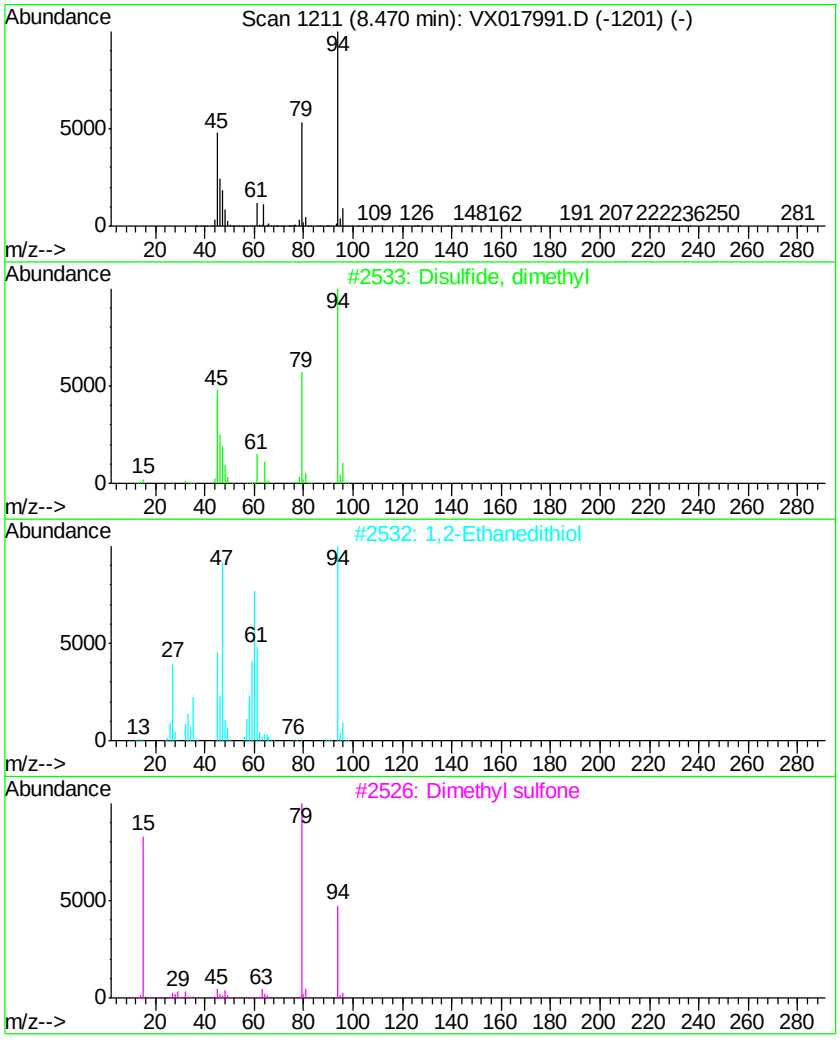
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

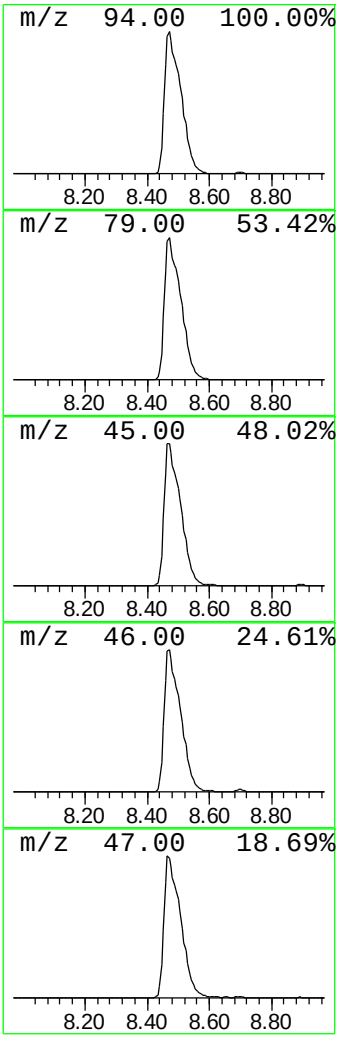
****

Peak Number 5 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	486.53 ug/l	18758800	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2	1,2-Ethanedithiol	94	C2H6S2	000540-63-6	58
3	Dimethyl sulfone	94	C2H6O2S	000067-71-0	46
4	Methanesulfonyl chloride	114	CH3ClO2S	000124-63-0	7
5	Methane, bromo-	94	CH3Br	000074-83-9	5





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Operator : JC/SP
Sample : L3721-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

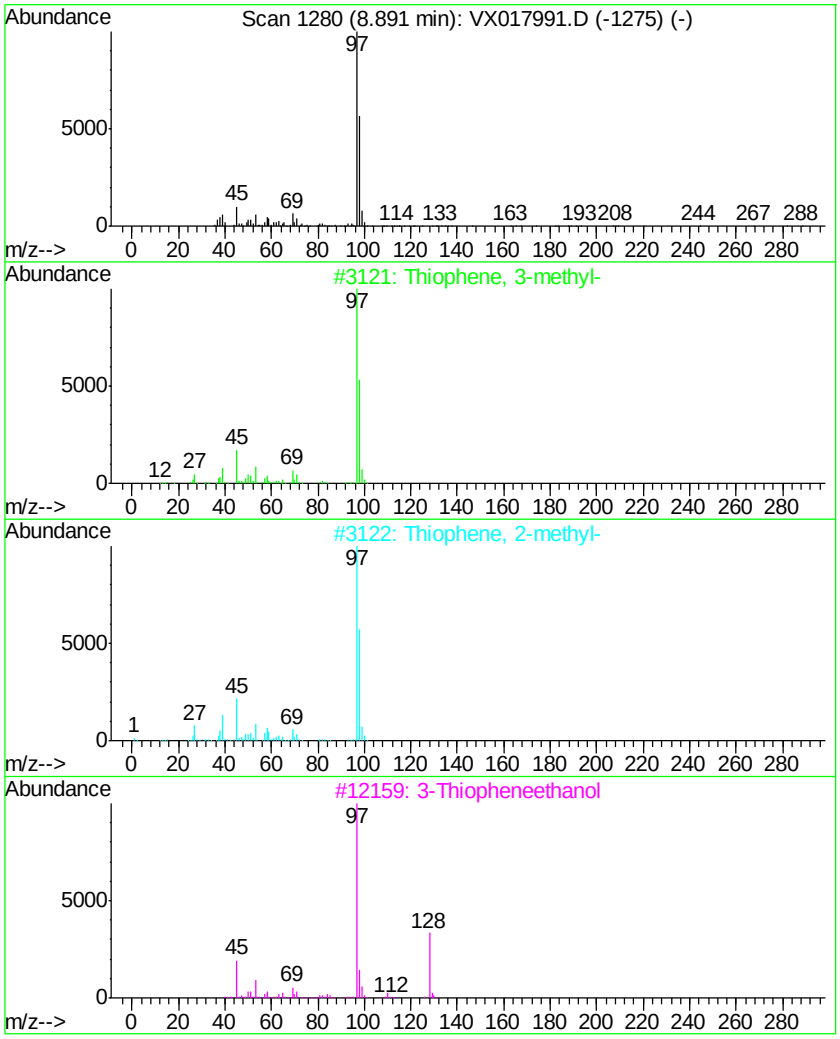
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

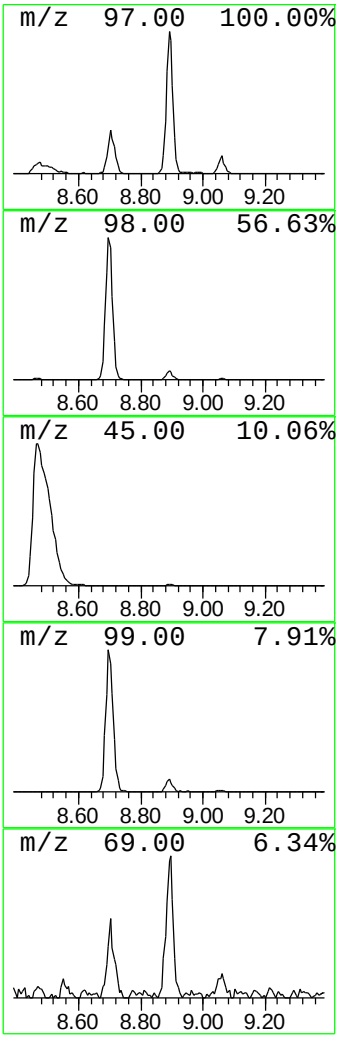
****

Peak Number 6 Thiophene, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.89	6.19 ug/l	238744	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 3-methyl-	98	C5H6S	000616-44-4	91
2	Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
3	3-Thiopheneethanol	128	C6H8OS	013781-67-4	53
4	2-Thiopheneethanol	128	C6H8OS	005402-55-1	36
5	Propennitrile, 3-ethoxy-2-(2-thi...	257	C10H11NO3S2	1000267-97-5	33





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Instrument : MSVOA_X
ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

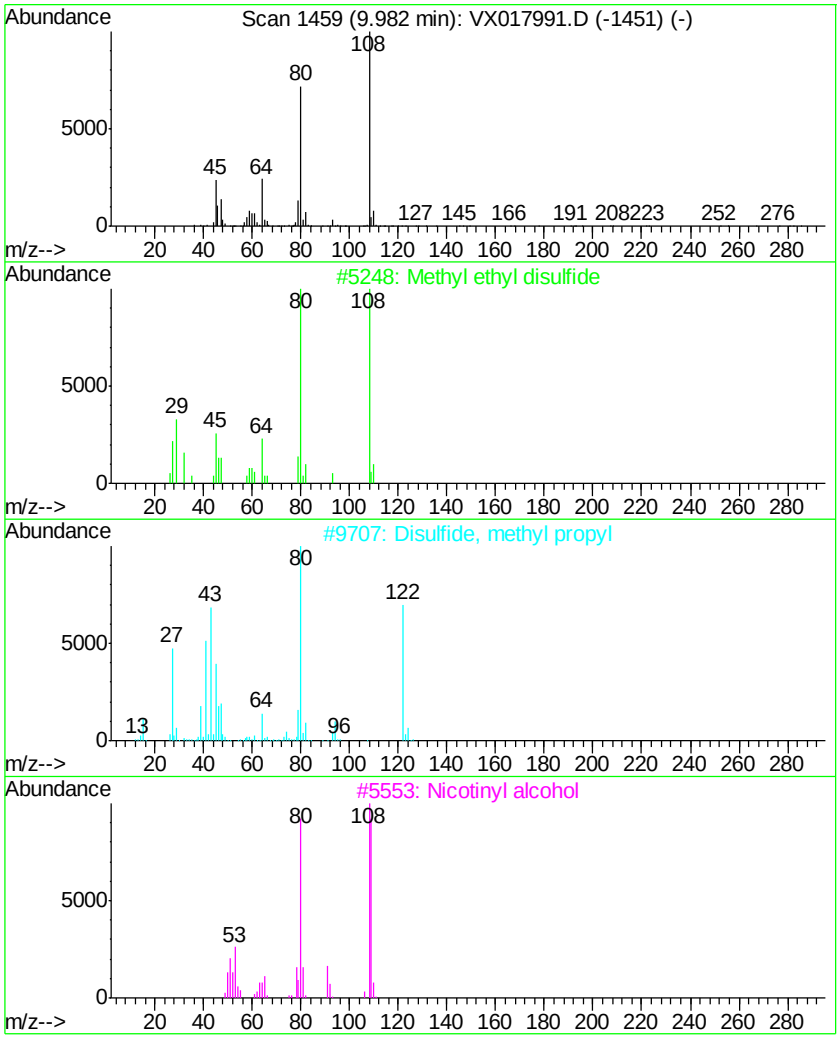
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

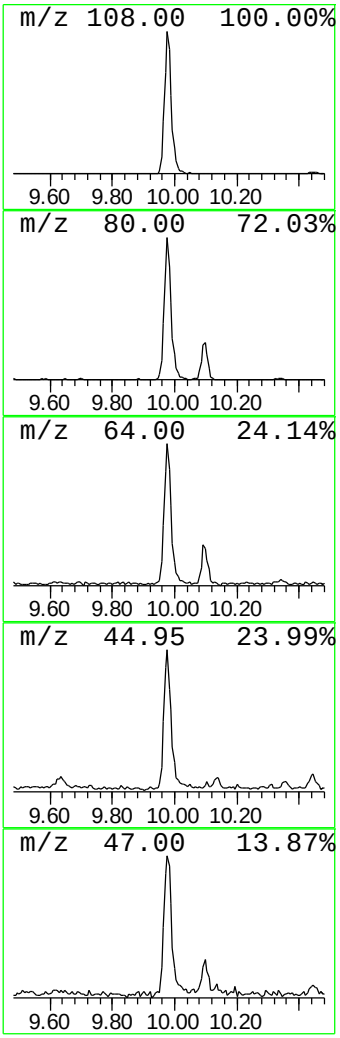
****

Peak Number 7 Methyl ethyl disulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.98	11.97 ug/l	461389	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	72
2	Disulfide, methyl propyl	122	C4H10S2	002179-60-4	64
3	Nicotinyl alcohol	109	C6H7NO	000100-55-0	64
4	Methyl n-butyl disulfide	136	C5H12S2	060779-24-0	59
5	Tris(ethanesulfonyl)methane	292	C7H16O6S3	021467-59-4	56





Library Search Compound Report

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ALS Vial : 22 Sample Multiplier: 1

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Quant Title : SW846 8260

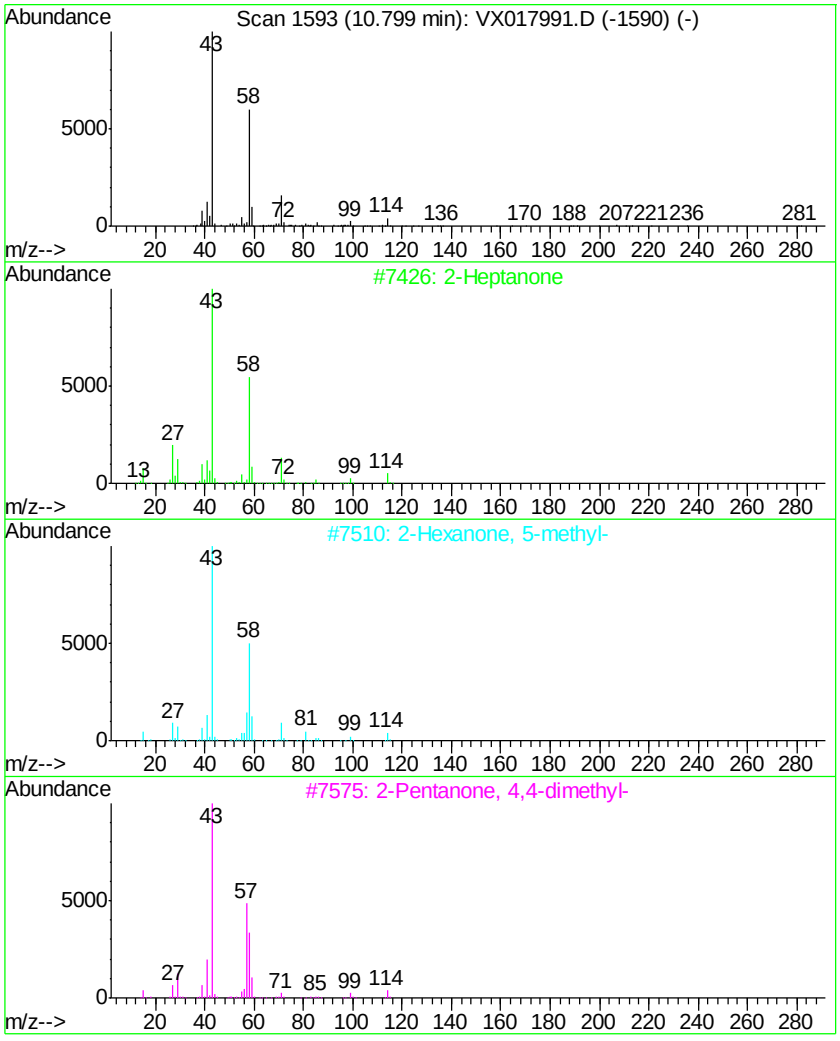
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

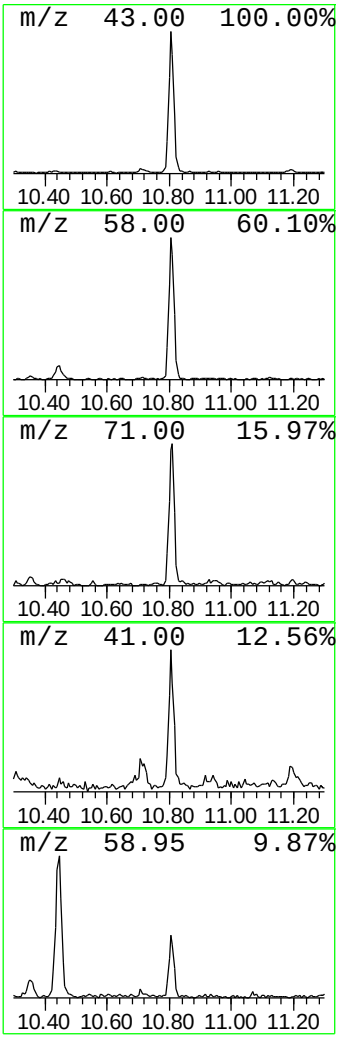
****

Peak Number 8 2-Heptanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.80	5.18 ug/l	199878	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	86
3	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	47
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	47
5	2-Nonanone	142	C9H18O	000821-55-6	40





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ClientSampleId : E-LGC-6

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

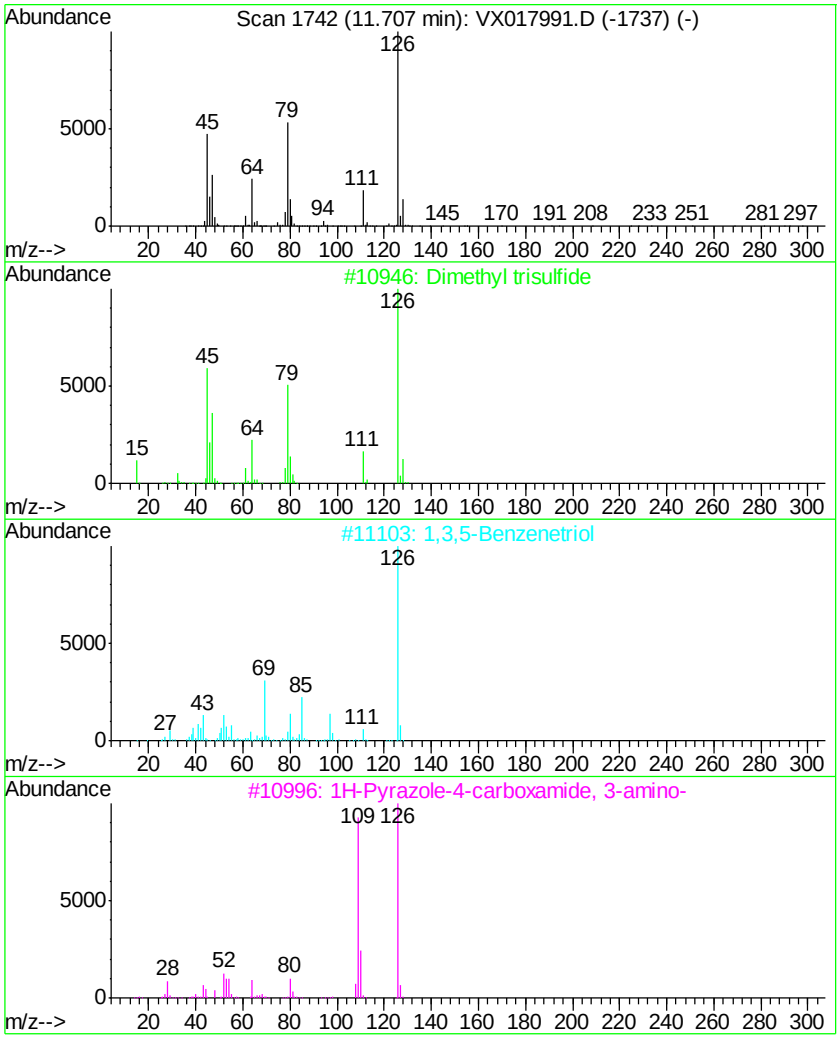
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

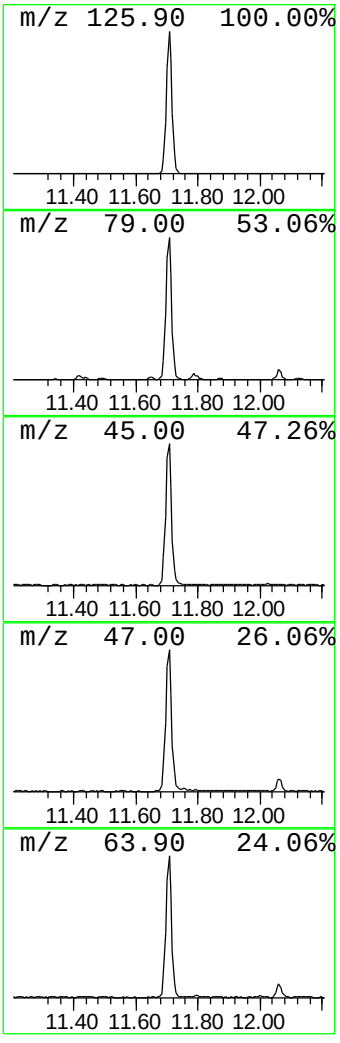
****

Peak Number 9 Dimethyl trisulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.71	26.86 ug/l	1016610	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl trisulfide	126	C2H6S3	003658-80-8	91
2	1,3,5-Benzenetriol	126	C6H6O3	000108-73-6	27
3	1H-Pyrazole-4-carboxamide, 3-amino-	126	C4H6N4O	005334-31-6	27
4	2,4,6-Trihydroxybenzoic acid	170	C7H6O5	000083-30-7	16
5	Dimethyldithiophosphinic acid	126	C2H7PS2	016367-68-3	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX081920\
Data File : VX017991.D
Acq On : 19 Aug 2020 17:36
Operator : JC/SP
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ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081920W.M
Quant Title : SW846 8260

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	1.26	46.5	ug/l	1274230	1	5.63	1368710	50.0
Aminomethanesulfo...	1.32	13.0	ug/l	356783	1	5.63	1368710	50.0
Methanethiol	1.57	231.5	ug/l	6335910	1	5.63	1368710	50.0
Ethanethiol	2.25	7.2	ug/l	197109	1	5.63	1368710	50.0
Disulfide, dimethyl	8.47	486.5	ug/l	18758800	3	10.10	1927830	50.0
Thiophene, 3-methyl-	8.89	6.2	ug/l	238744	3	10.10	1927830	50.0
Methyl ethyl disu...	9.98	12.0	ug/l	461389	3	10.10	1927830	50.0
2-Heptanone	10.80	5.2	ug/l	199878	3	10.10	1927830	50.0
Dimethyl trisulfide	11.71	26.9	ug/l	1016610	4	12.06	1892160	50.0