LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082020\
Data File : VX018035.D
Acq On : 20 Aug 2020 15:19
Operator : JC/SP
Sample : L3721-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : I-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	1.179	12	15	23	rVV	103375	107128	2.77%	0.425%
2	1.246	23	26	35	rVB	199097	209039	5.40%	0.829%
3	1.471	52	63	66	rBV3	55865	173343	4.48%	0.688%
4	1.569	76	79	94	rBV	494823	726062	18.76%	2.881%
5	2.087	160	164	171	rBV	52915	86278	2.23%	0.342%
6	2.252	185	191	198	rBV	27822	50110	1.29%	0.199%
7	2.422	212	219	223	rBV	1477703	2413346	62.36%	9.575%
8	2.459	223	225	233	rVB	288441	435694	11.26%	1.729%
9	2.550	234	240	244	rBV	526341	932855	24.10%	3.701%
10	4.641	573	583	593	rBV2	75638	229849	5.94%	0.912%
11	5.105	651	659	665	rBV4	19659	59528	1.54%	0.236%
12	5.471	708	719	731	rBV2	358836	1036339	26.78%	4.112%
13	5.635	731	746	761	rBV	633740	1773192	45.82%	7.035%
14	6.031	798	811	820	rBV	392752	1036267	26.78%	4.112%
15	6.117	820	825	833	rVB2	31572	80213	2.07%	0.318%
16	6.836	932	943	964	rBV3	1021314	3870237	100.00%	15.356%
17	7.135	987	992	1013	rVB2	152860	511979	13.23%	2.031%
18	8.464	1203	1210	1220	rBV2	222763	432528	11.18%	1.716%
19	8.696	1241	1248	1256	rBV	1916199	2993298	77.34%	11.876%
20	8.891	1276	1280	1285	rVB3	30999	48671	1.26%	0.193%
21	9.976	1453	1458	1465	rVB	42438	65680	1.70%	0.261%
22	10.098	1472	1478	1489	rVB	1952450	2625557	67.84%	10.417%
23	11.122	1640	1646	1655	rVB	1695057	2074830	53.61%	8.232%
24	11.701	1732	1741	1752	rBV	100527	146762	3.79%	0.582%
25	12.061	1795	1800	1807	rVB	2189819	2623435	67.78%	10.409%
26	12.945	1941	1945	1949	rBV	43970	53436	1.38%	0.212%
27	13.554	2040	2045	2051	rVB	50863	66644	1.72%	0.264%
28	13.652	2052	2061	2063	rBV9	13889	40947	1.06%	0.162%
29	13.817	2083	2088	2094	rBV	200165	255928	6.61%	1.015%
30	15.676	2391	2393	2401	rVB7	20868	44794	1.16%	0.178%

Sum of corrected areas: 25203969

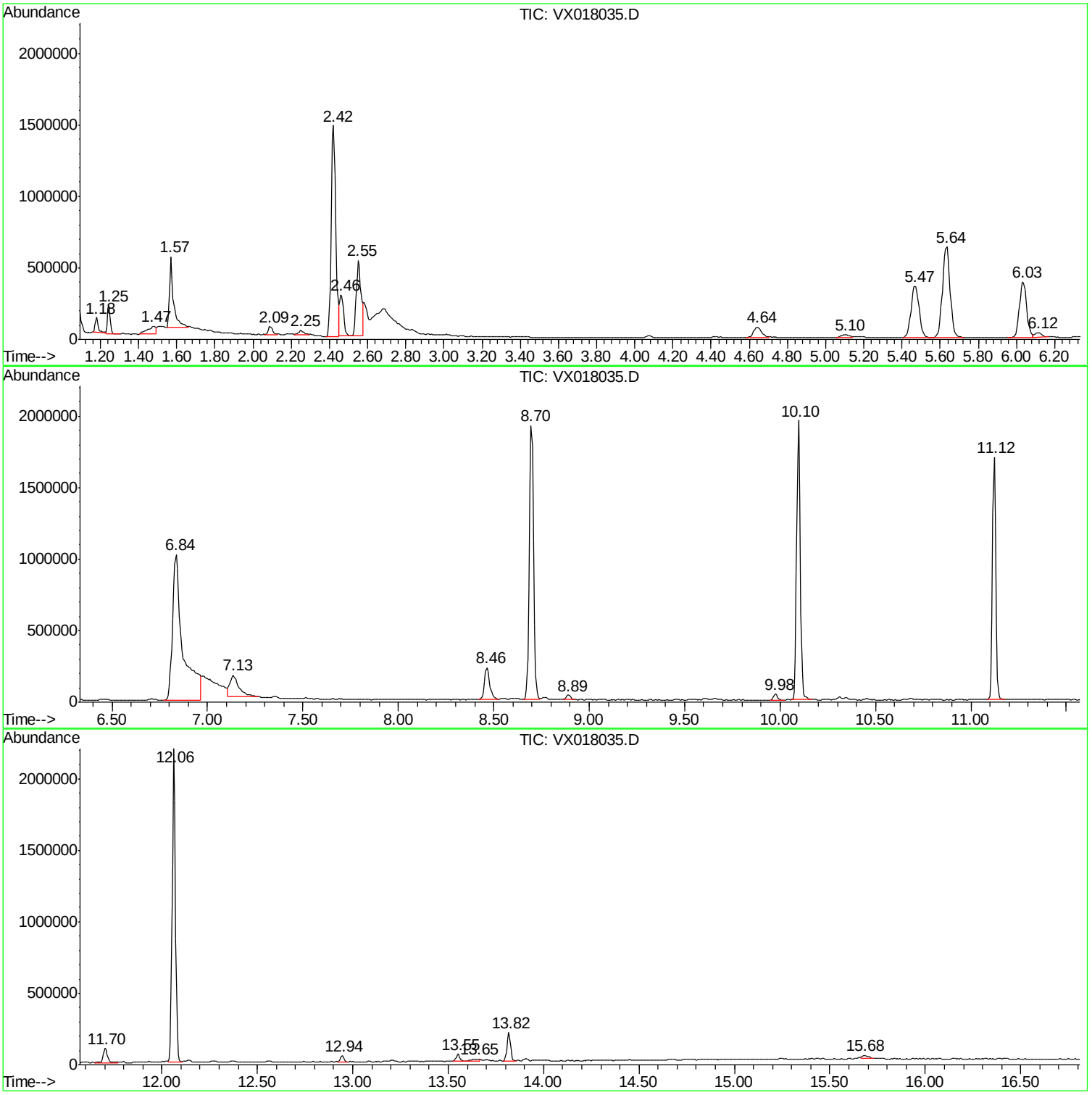
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX082020\
Data File : VX018035.D
Acq On : 20 Aug 2020 15:19
Operator : JC/SP
Sample : L3721-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : I-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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018035.D
Acq On : 20 Aug 2020 15:19
Operator : JC/SP
Sample : L3721-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : I-LGC-6

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

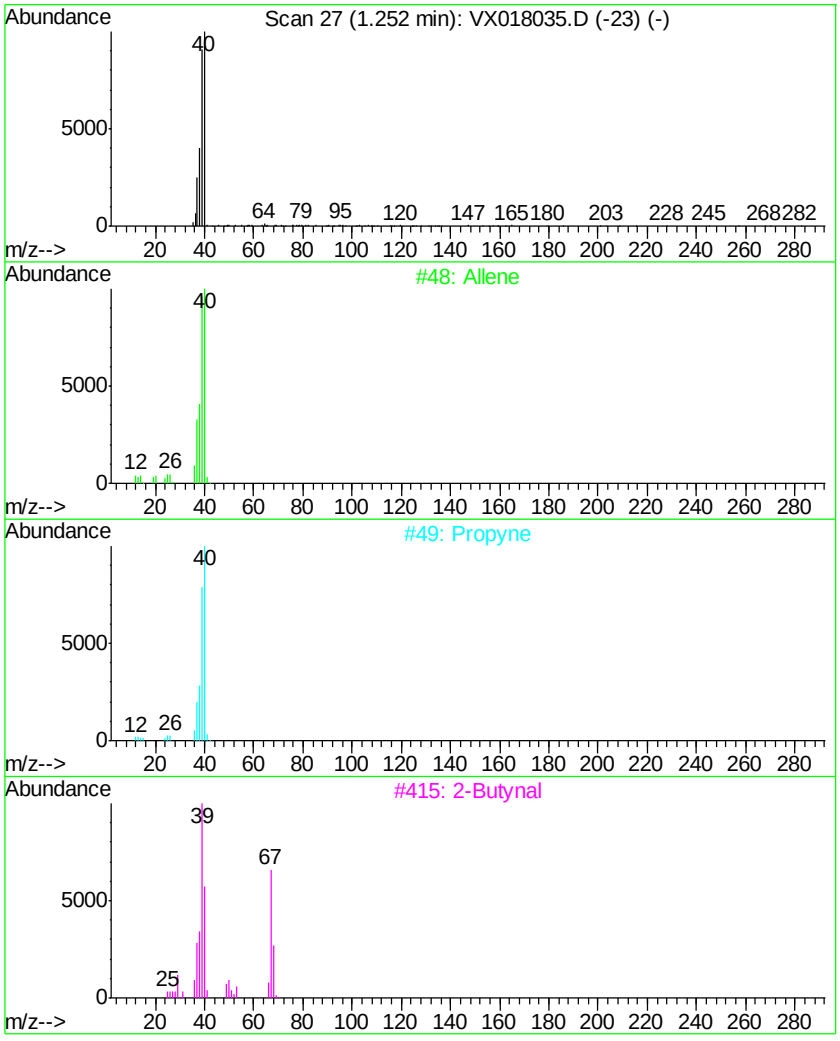
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

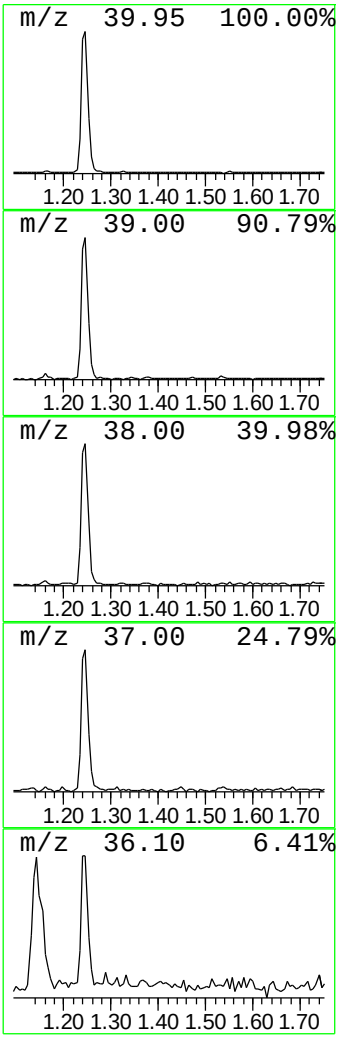
****

Peak Number 1 Allene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.25	5.89 ug/l	209039	Pentafluorobenzene	5.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allene	40	C3H4	000463-49-0	90
2	Propyne	40	C3H4	000074-99-7	90
3	2-Butynal	68	C4H4O	001119-19-3	74
4	3-Butyn-1-ol	70	C4H6O	000927-74-2	74
5	Thiocyanic acid, 2-propynyl ester	97	C4H3NS	024309-48-6	64





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018035.D
Acq On : 20 Aug 2020 15:19
Operator : JC/SP
Sample : L3721-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : I-LGC-6

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

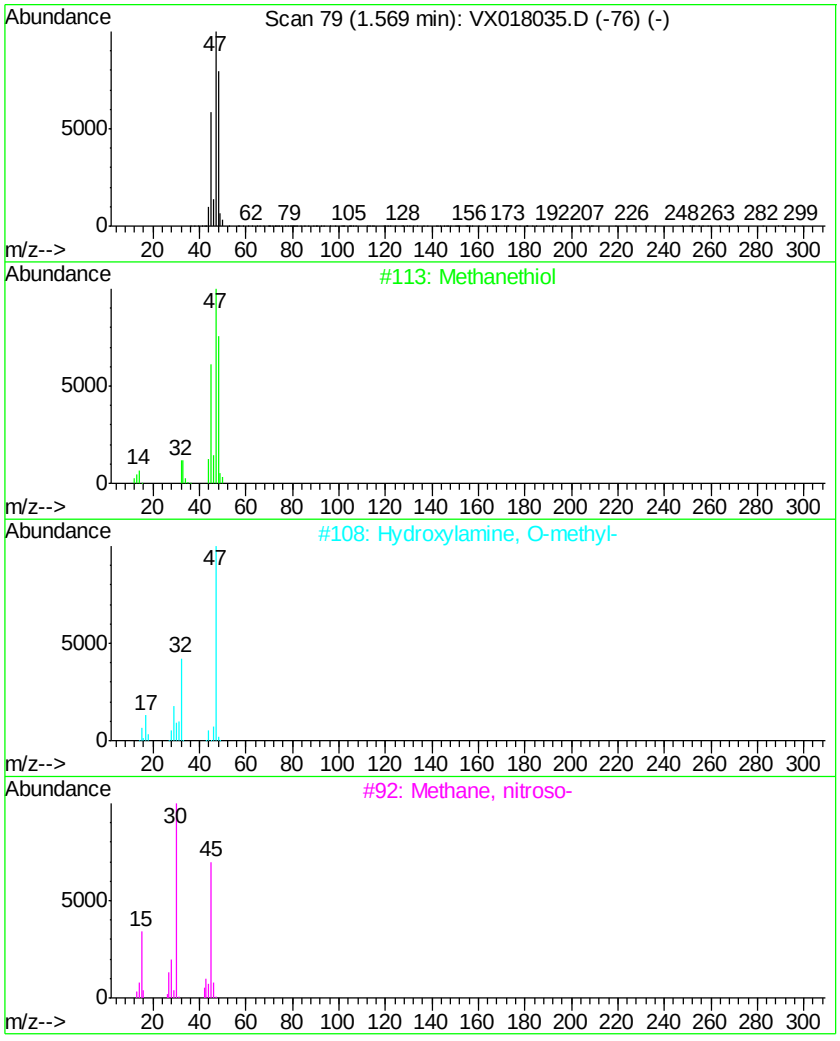
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

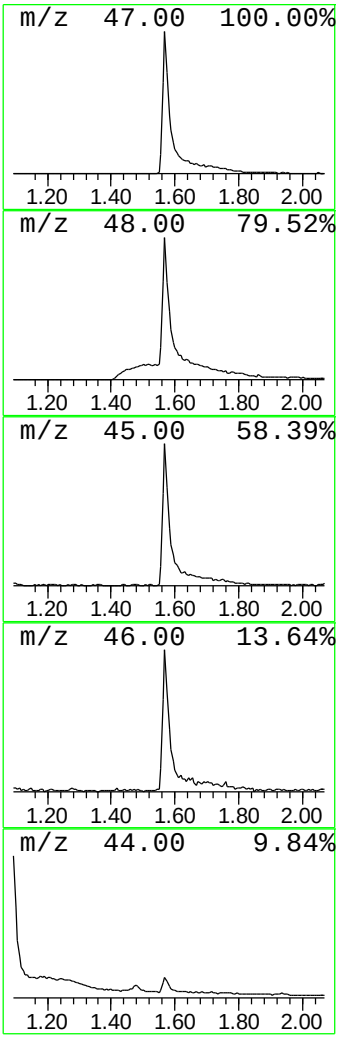
****

Peak Number 2 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.57	20.47 ug/l	726062	Pentafluorobenzene	5.64

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\VX082020\
Data File : VX018035.D
Acq On : 20 Aug 2020 15:19
Operator : JC/SP
Sample : L3721-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : I-LGC-6

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

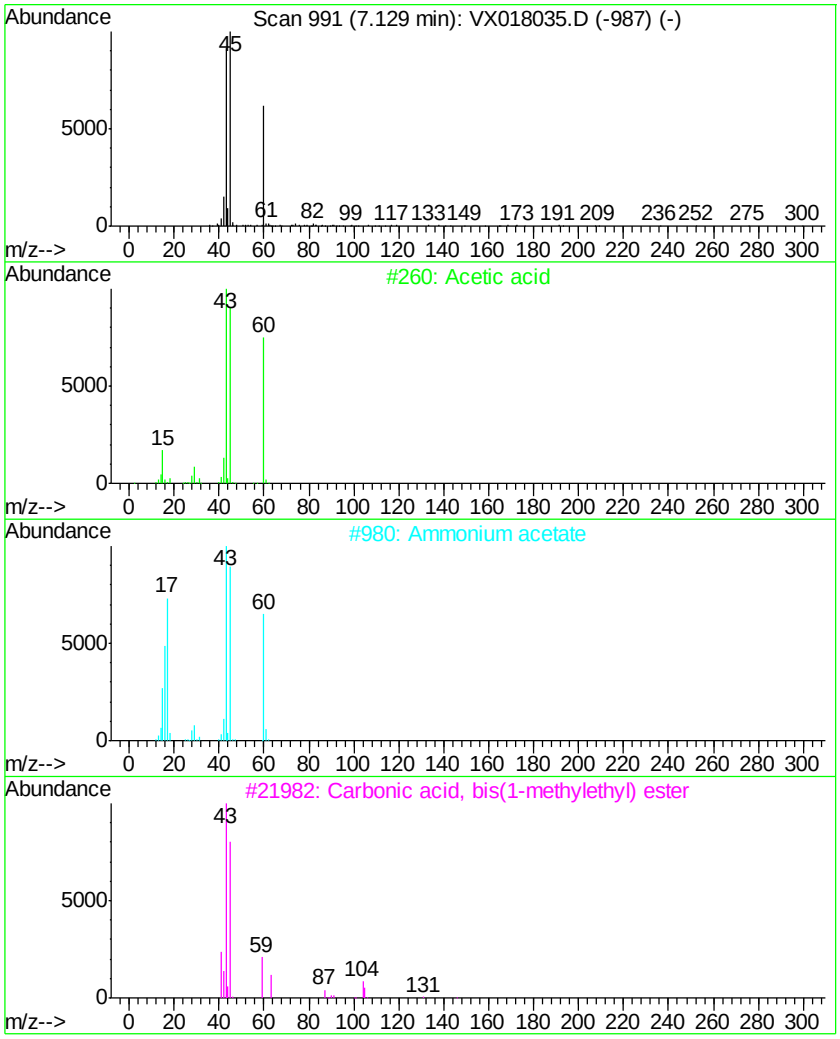
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

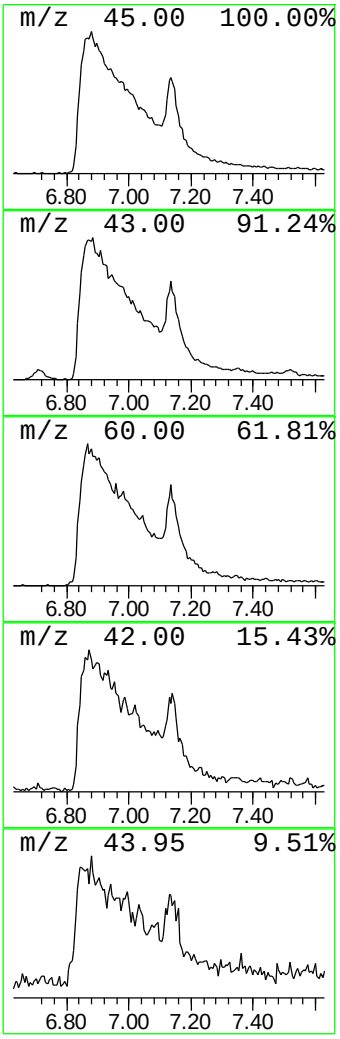
****

Peak Number 3 Acetic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	6.61 ug/l	511979	1,4-Difluorobenzene	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	86
2	Ammonium acetate	77	C2H7NO2	000631-61-8	78
3	Carbonic acid, bis(1-methylethyl...	146	C7H14O3	006482-34-4	53
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	16





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018035.D
Acq On : 20 Aug 2020 15:19
Operator : JC/SP
Sample : L3721-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : I-LGC-6

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

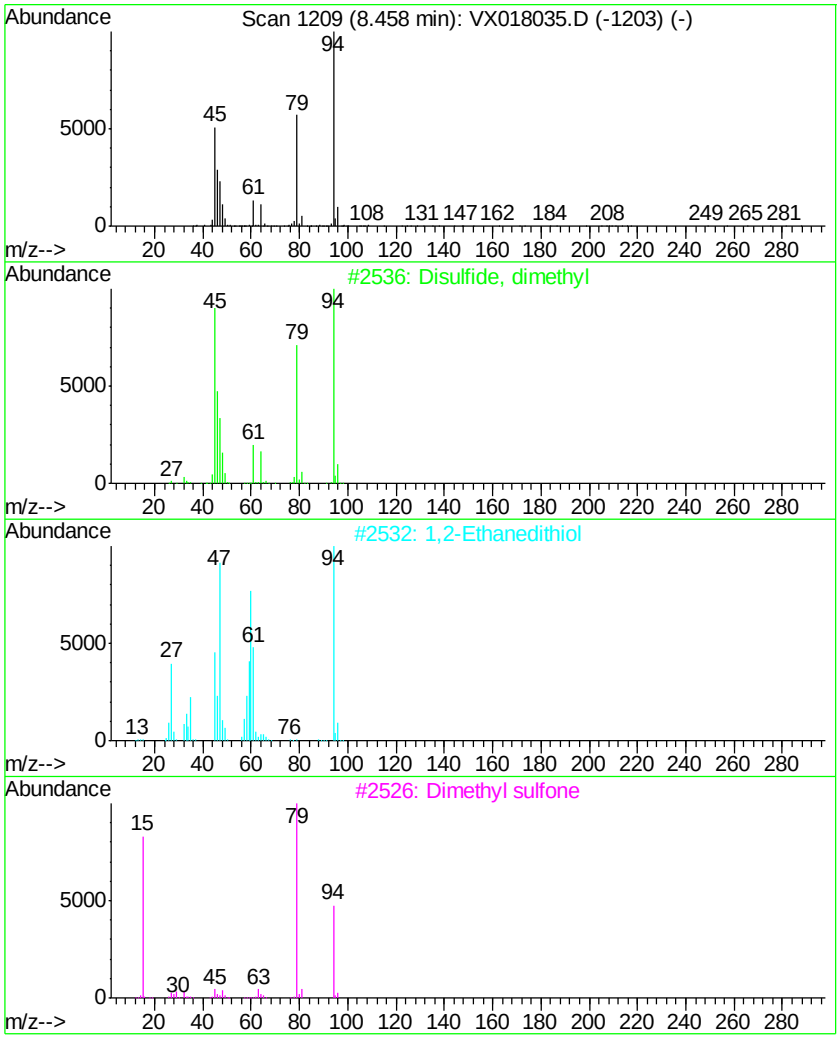
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

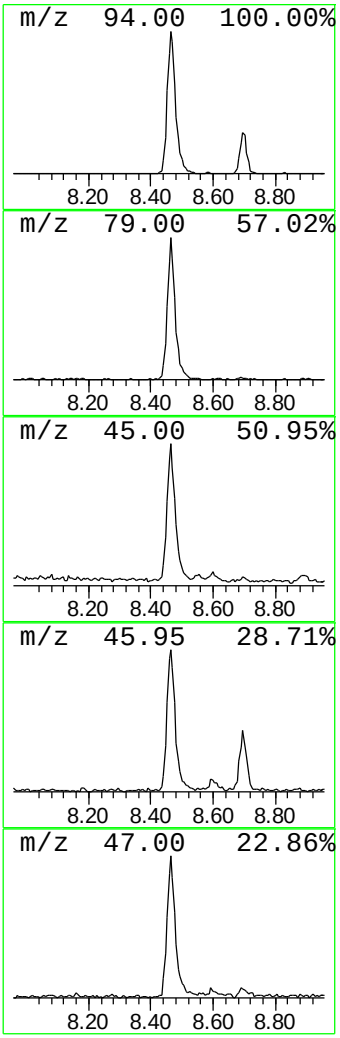
****

Peak Number 4 Disulfide, dimethyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	5.59 ug/l	432528	1,4-Difluorobenzene	6.84

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	52
3	Dimethyl sulfone	94	C2H6O2S	000067-71-0	46
4	1,2,3,6-Tetrahydrobenzylalcohol,...	126	C8H14O	1000365-07-7	9
5	Dimethyl methylphosphonate	124	C3H9O3P	000756-79-6	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX082020\
Data File : VX018035.D
Acq On : 20 Aug 2020 15:19
Operator : JC/SP
Sample : L3721-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : I-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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Allene	1.25	5.9	ug/l	209039	1	5.64	1773190	50.0
Methanethiol	1.57	20.5	ug/l	726062	1	5.64	1773190	50.0
Acetic acid	7.13	6.6	ug/l	511979	2	6.84	3870240	50.0
Disulfide, dimethyl	8.46	5.6	ug/l	432528	2	6.84	3870240	50.0