LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV012420\
Data File : VV014392.D
Acq On : 24 Jan 2020 16:00
Operator : SY/MD
Sample : L1253-02MS
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : H0AB0MS

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\SOMVTR010220WMA.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	1.319	63	71	85	rVB2	442575	486804	1.39%	0.457%
2	1.479	113	121	147	rBV	4488589	6341631	18.06%	5.954%
3	1.582	148	153	171	rVB	358000	586805	1.67%	0.551%
4	2.135	315	325	343	rVB4	1024531	1682485	4.79%	1.580%
5	2.232	345	355	372	rVB	632352	995108	2.83%	0.934%
6	2.537	442	450	475	rVB2	401533	808860	2.30%	0.759%
7	3.958	874	892	941	rBV	14193988	35106334	100.00%	32.962%
8	4.399	1013	1029	1053	rVB	557168	1360517	3.88%	1.277%
9	5.093	1227	1245	1253	rBV2	1214930	2892310	8.24%	2.716%
10	5.145	1254	1261	1287	rVB	1474240	3076161	8.76%	2.888%
11	5.659	1410	1421	1446	rVB	1107531	2202191	6.27%	2.068%
12	5.955	1496	1513	1547	rBV	13409606	25637921	73.03%	24.072%
13	6.113	1550	1562	1580	rVB	734707	1474673	4.20%	1.385%
14	7.026	1834	1846	1860	rBV	379283	691722	1.97%	0.649%
15	7.129	1867	1878	1898	rBV	208117	447762	1.28%	0.420%
16	7.357	1936	1949	1960	rBV	1315513	2288360	6.52%	2.149%
17	7.428	1960	1971	1994	rVB	2163370	3696183	10.53%	3.470%
18	7.662	2029	2044	2065	rBV	223271	421279	1.20%	0.396%
19	8.132	2179	2190	2228	rBV	1809625	3667549	10.45%	3.444%
20	8.891	2412	2426	2430	rBV	1685260	2567163	7.31%	2.410%
21	8.920	2431	2435	2451	rVB	1857172	2712728	7.73%	2.547%
22	10.254	2839	2850	2866	rBV	542303	868227	2.47%	0.815%
23	10.833	3019	3030	3046	rBV	347474	606849	1.73%	0.570%
24	10.977	3057	3075	3090	rBV	683571	1110890	3.16%	1.043%
25	11.289	3160	3172	3192	rBV	1694764	2594629	7.39%	2.436%
26	11.666	3278	3289	3308	rVB	1418876	2181260	6.21%	2.048%

Sum of corrected areas: 106506401

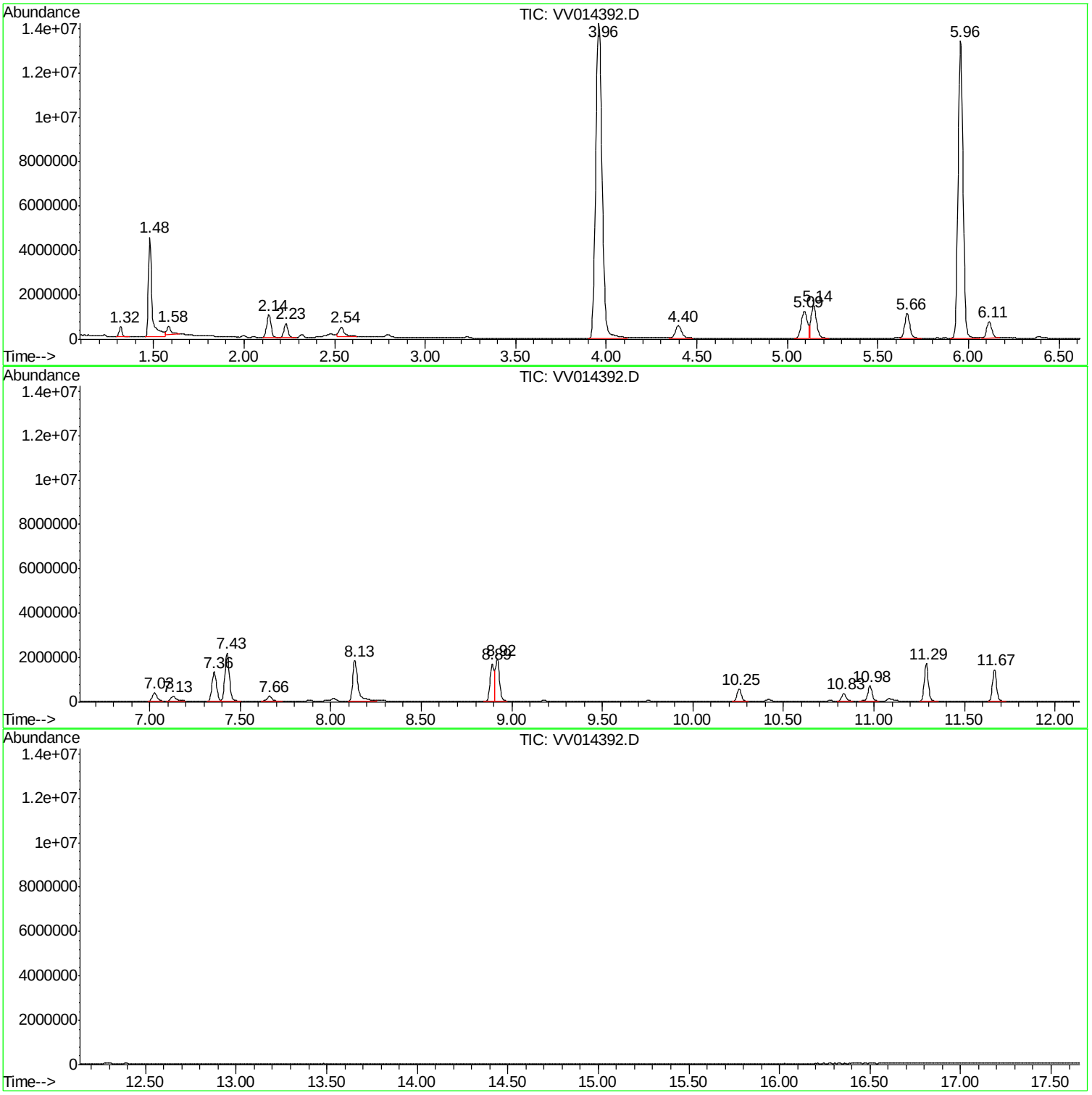
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV012420\
Data File : VV014392.D
Acq On : 24 Jan 2020 16:00
Operator : SY/MD
Sample : L1253-02MS
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : H0AB0MS

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
Quant Title : TRACE VOA SOM01.0

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV012420\
Data File : VV014392.D
Acq On : 24 Jan 2020 16:00
Operator : SY/MD
Sample : L1253-02MS
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : H0AB0MS

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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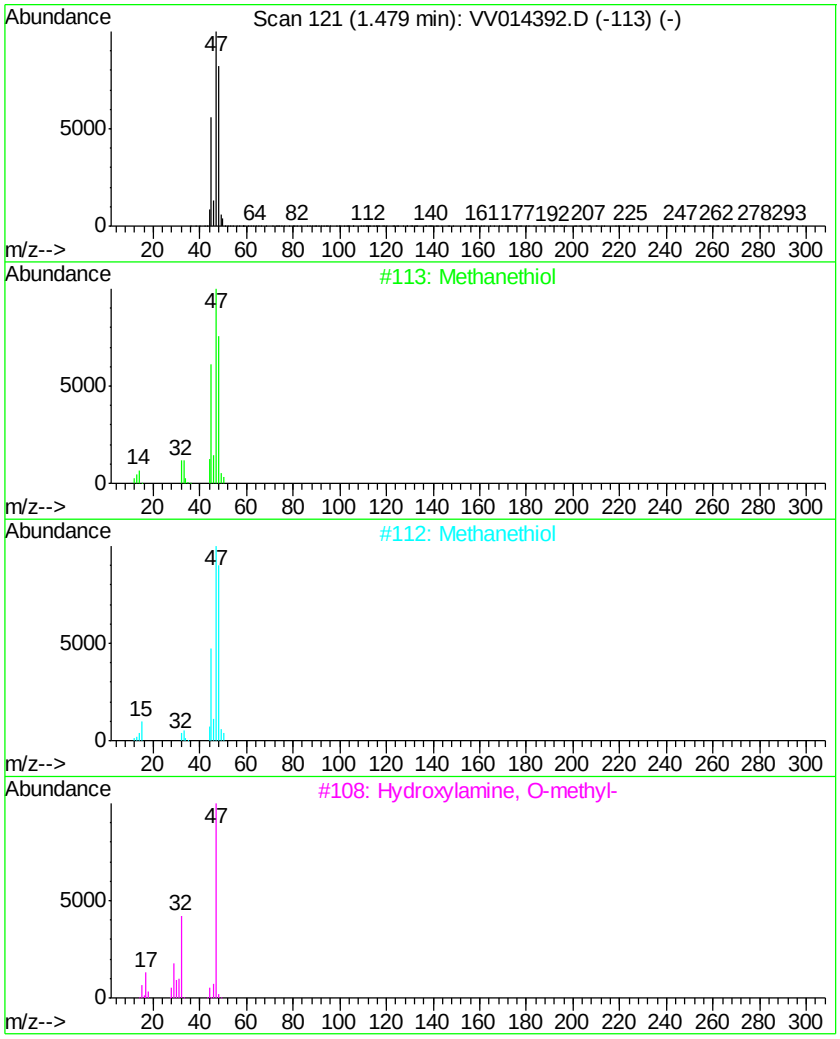
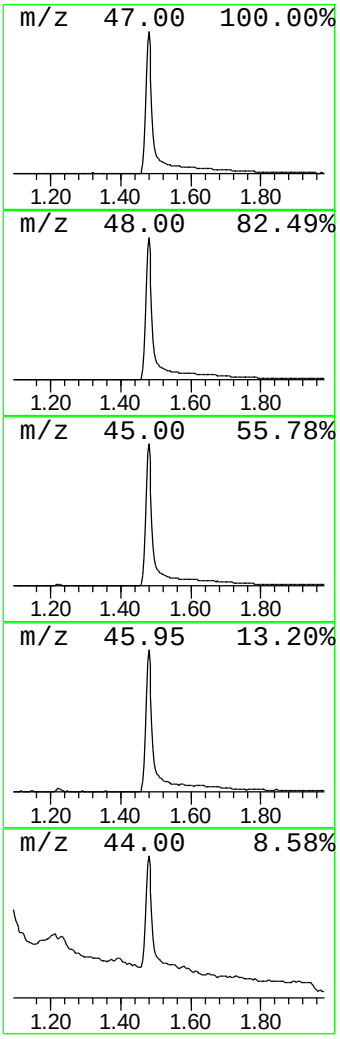
Peak Number 1 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	14.40 ug/L	6341630	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	90
2	Methanethiol	48	CH4S	000074-93-1	90
3	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5	Methane, nitroso-	45	CH3NO	000865-40-7	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV012420\
Data File : VV014392.D
Acq On : 24 Jan 2020 16:00
Operator : SY/MD
Sample : L1253-02MS
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : H0AB0MS

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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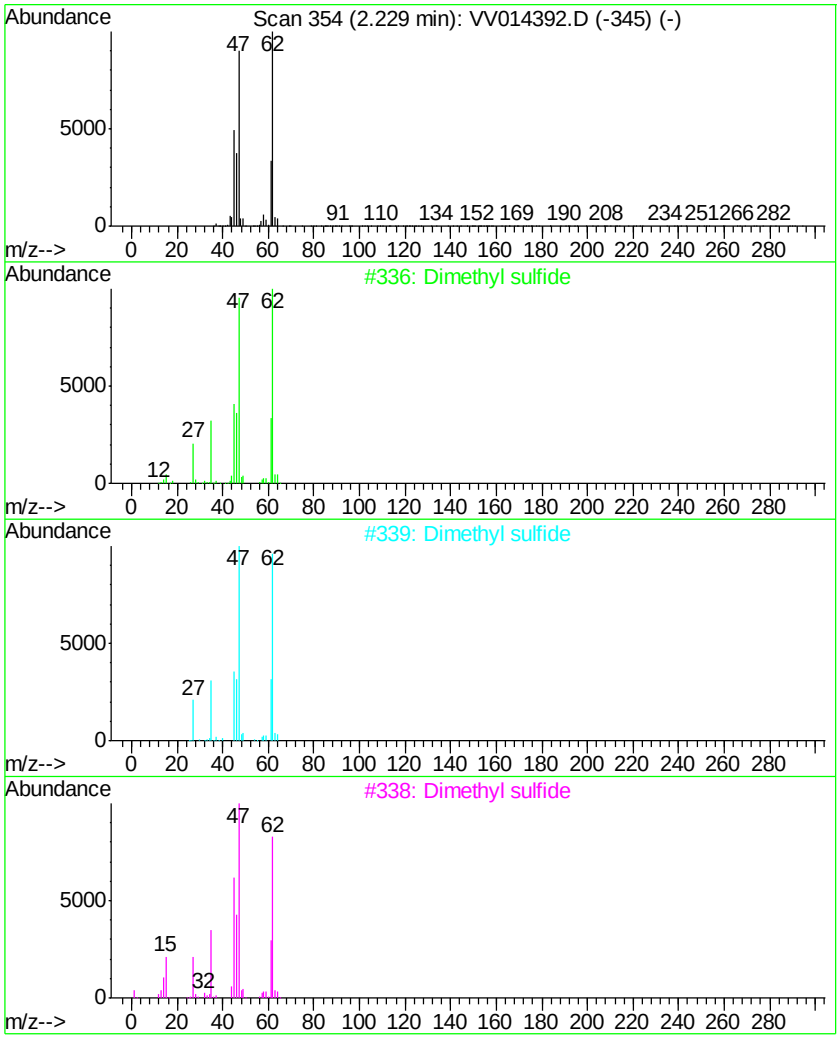
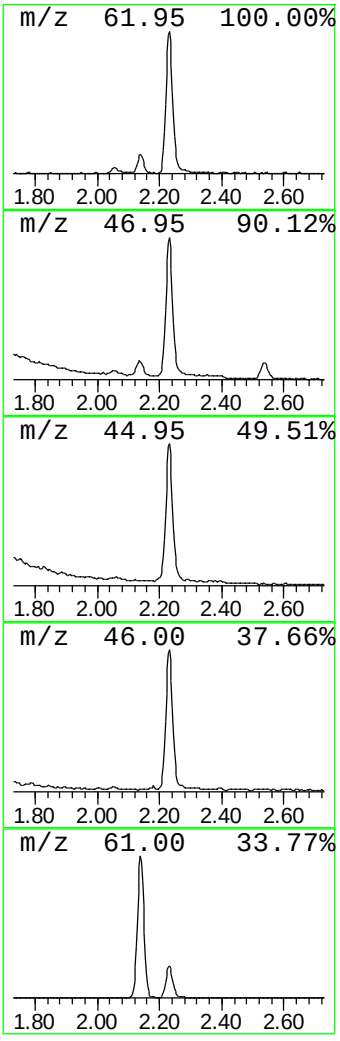
Peak Number 2 Dimethyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.23	2.26 ug/L	995108	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Dimethyl sulfide	62	C2H6S	000075-18-3	91
3	Dimethyl sulfide	62	C2H6S	000075-18-3	91
4	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
5	Dimethyl sulfide	62	C2H6S	000075-18-3	87





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV012420\
Data File : VV014392.D
Acq On : 24 Jan 2020 16:00
Operator : SY/MD
Sample : L1253-02MS
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : H0AB0MS

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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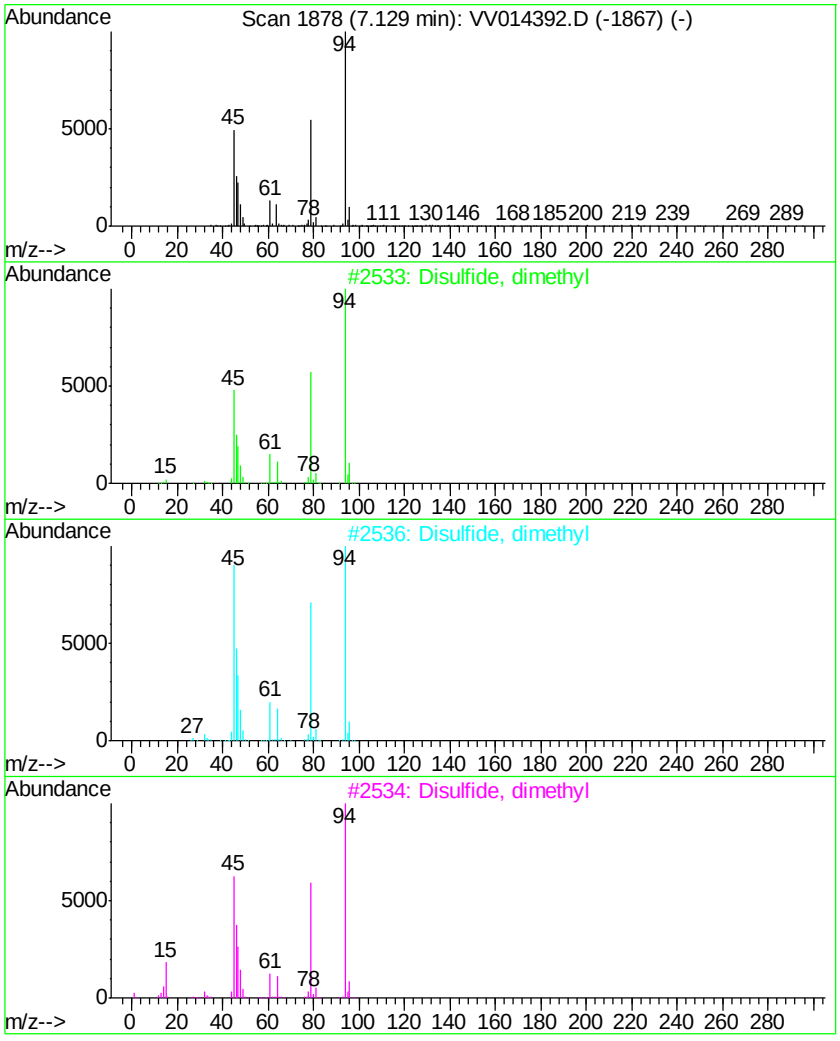
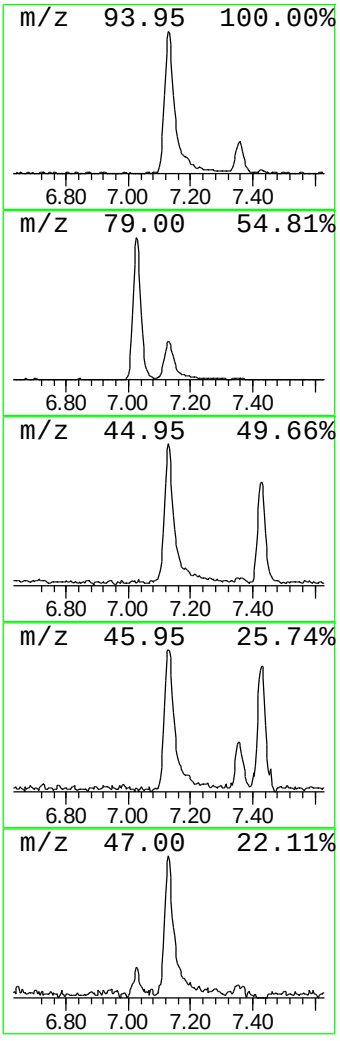
Peak Number 4 Disulfide, dimethyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.13	1.02 ug/L	447762	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
4	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV012420\
Data File : VV014392.D
Acq On : 24 Jan 2020 16:00
Operator : SY/MD
Sample : L1253-02MS
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : H0AB0MS

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
Quant Title : TRACE VOA SOM01.0

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

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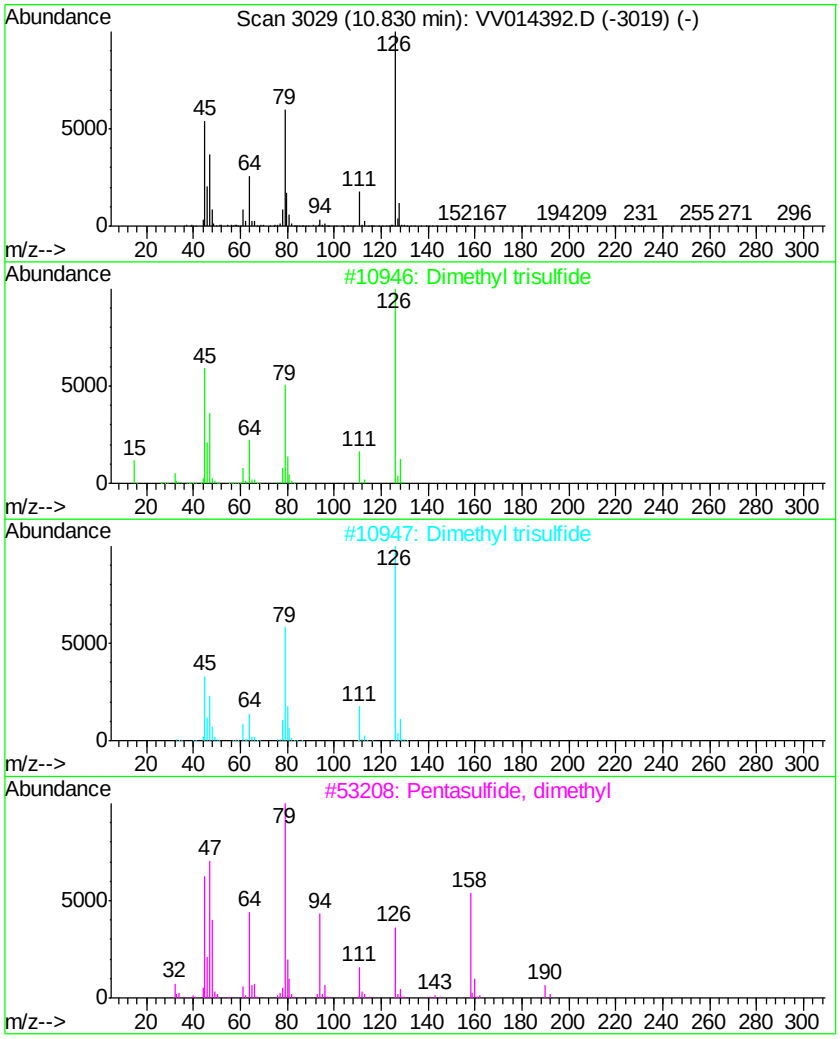
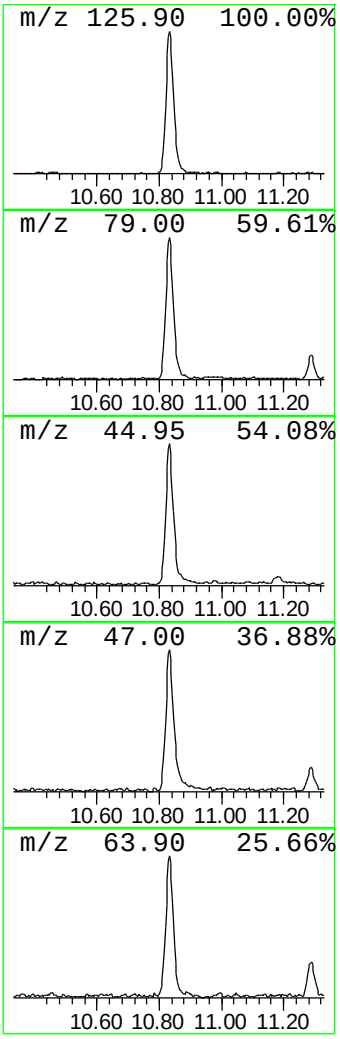
Peak Number 5 Dimethyl trisulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	1.17 ug/L	606849	1,4-Dichlorobenzene-d4	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl trisulfide	126	C2H6S3	003658-80-8	96
2	Dimethyl trisulfide	126	C2H6S3	003658-80-8	81
3	Pentasulfide, dimethyl	190	C2H6S5	007330-31-6	32
4	Phosphonic acid, (3-methyl-2-oxo...	206	C8H15O4P	054543-04-3	25
5	S-(2,2,2-Trifluoroethyl) methane...	194	C3H5F3O2S2	069466-44-0	23





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Data File : VV014392.D
Acq On : 24 Jan 2020 16:00
Operator : SY/MD
Sample : L1253-02MS
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : H0AB0MS

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
Quant Title : TRACE VOA SOM01.0

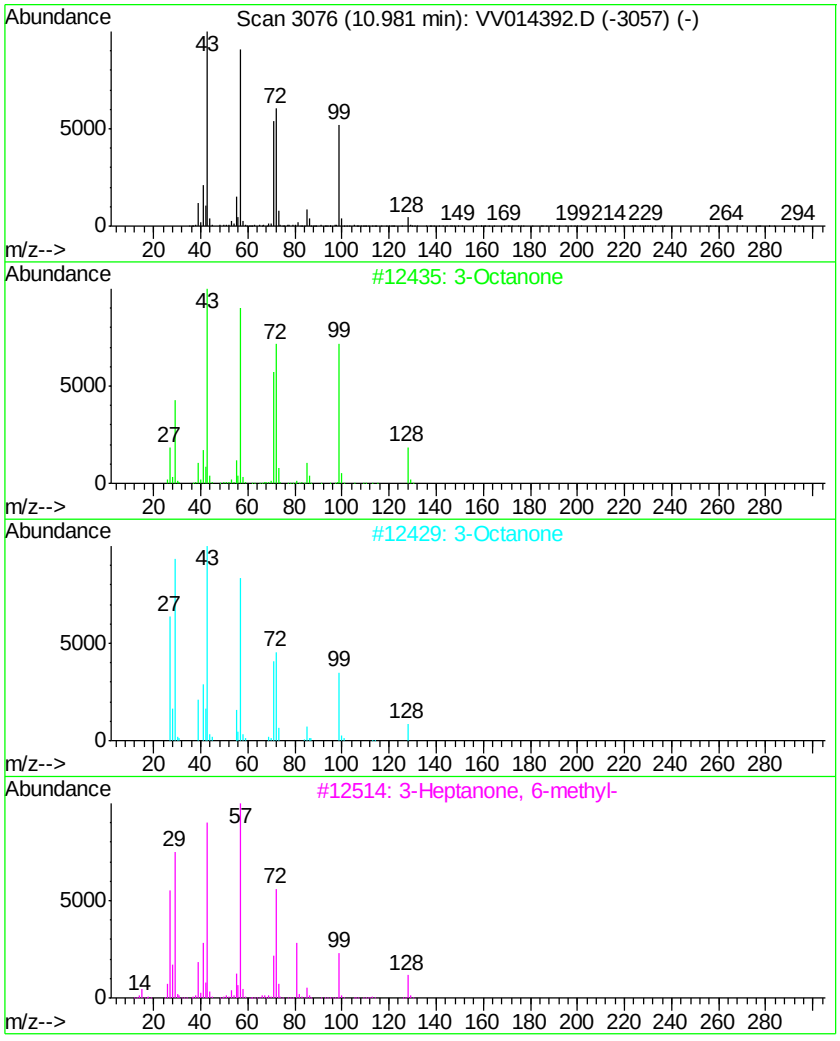
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

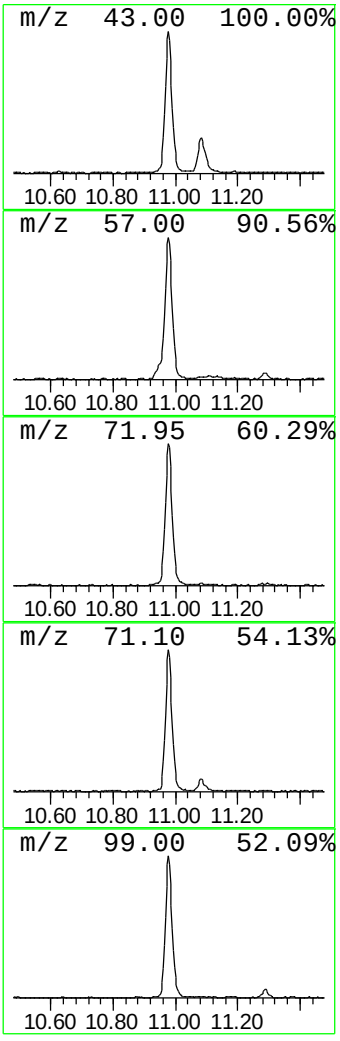
****

Peak Number 6 3-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	2.14 ug/L	1110890	1,4-Dichlorobenzene-d4	11.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	94
2	3-Octanone	128	C8H16O	000106-68-3	74
3	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	58
4	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	49
5	3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	47





Tentatively Identified Compound (LSC) summary

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Data File : VV014392.D
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ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId : H0AB0MS

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR010220WMA.M
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
Methanethiol	1.48	14.4	ug/L	6341630	1	5.66	2202190	5.0
Dimethyl sulfide	2.23	2.3	ug/L	995108	1	5.66	2202190	5.0
Disulfide, dimethyl	7.13	1.0	ug/L	447762	1	5.66	2202190	5.0
Dimethyl trisulfide	10.83	1.2	ug/L	606849	3	11.29	2594630	5.0
3-Octanone	10.98	2.1	ug/L	1110890	3	11.29	2594630	5.0