LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV071918\
Data File : VV006645.D
Acq On : 19 Jul 2018 16:21
Operator : SY/MD
Sample : J3983-19
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

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\SOMVTR071918WMA.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	1.028	24	43	59	rBV	3986286	5034518	48.64%	16.933%
2	1.257	106	114	124	rBV	116732	315111	3.04%	1.060%
3	1.321	129	134	141	rVB2	179074	213669	2.06%	0.719%
4	1.479	175	183	211	rBV	6476965	10351269	100.00%	34.814%
5	2.054	353	362	377	rBV	1098637	1524712	14.73%	5.128%
6	2.131	378	386	399	rVB	244839	353441	3.41%	1.189%
7	2.231	403	417	433	rVB2	400483	691859	6.68%	2.327%
8	2.466	480	490	504	rBV	678716	1138832	11.00%	3.830%
9	2.790	582	591	604	rVB	149999	250736	2.42%	0.843%
10	3.961	939	955	971	rBV	135672	361033	3.49%	1.214%
11	4.044	972	981	1002	rVB	49764	128105	1.24%	0.431%
12	4.405	1075	1093	1119	rBV	163433	393835	3.80%	1.325%
13	5.099	1291	1309	1324	rBV2	396527	912113	8.81%	3.068%
14	5.668	1471	1486	1501	rBV	317107	668685	6.46%	2.249%
15	6.122	1617	1627	1645	rVB	224628	447003	4.32%	1.503%
16	6.658	1784	1794	1815	rVB	62884	116750	1.13%	0.393%
17	7.035	1898	1911	1926	rBV	97708	172476	1.67%	0.580%
18	7.138	1928	1943	1975	rBV	796280	1428584	13.80%	4.805%
19	7.363	2000	2013	2027	rBV	467417	785764	7.59%	2.643%
20	7.668	2097	2108	2125	rBV	64982	112992	1.09%	0.380%
21	8.141	2241	2255	2287	rBV	588573	1025368	9.91%	3.449%
22	8.758	2435	2447	2466	rBV	115267	199570	1.93%	0.671%
23	8.900	2473	2491	2523	rBV	467562	908694	8.78%	3.056%
24	10.266	2905	2916	2931	rVB	168328	259130	2.50%	0.872%
25	10.842	3083	3095	3125	rVB	121847	211952	2.05%	0.713%
26	11.089	3154	3172	3184	rBV	121299	194845	1.88%	0.655%
27	11.301	3226	3238	3258	rBV	427821	672371	6.50%	2.261%
28	11.678	3342	3355	3379	rVB	423979	676921	6.54%	2.277%
29	12.285	3533	3544	3552	rBV	116669	182445	1.76%	0.614%

Sum of corrected areas: 29732783

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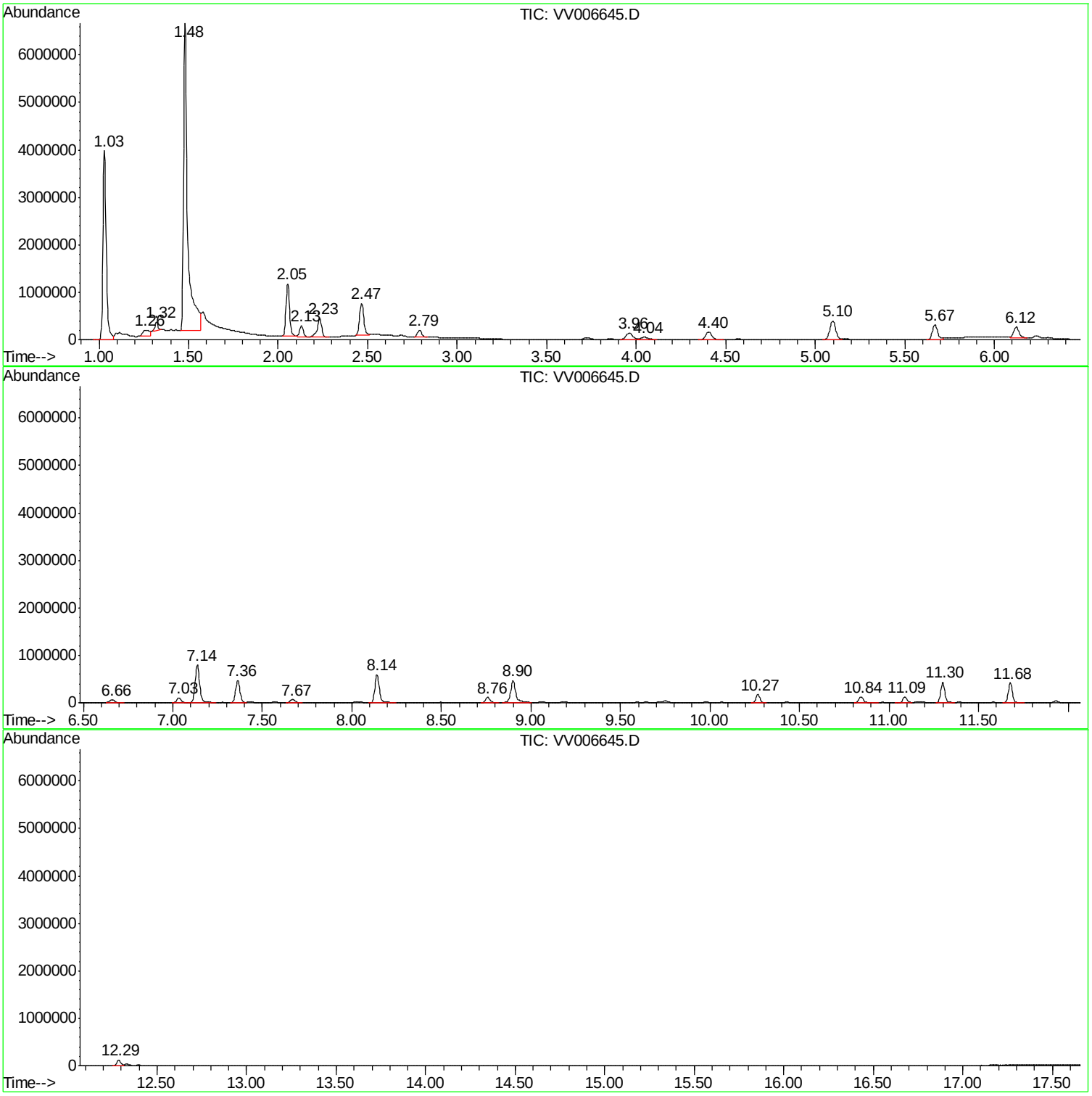
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

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



Library Search Compound Report

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Data File : VV006645.D
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Operator : SY/MD
Sample : J3983-19
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

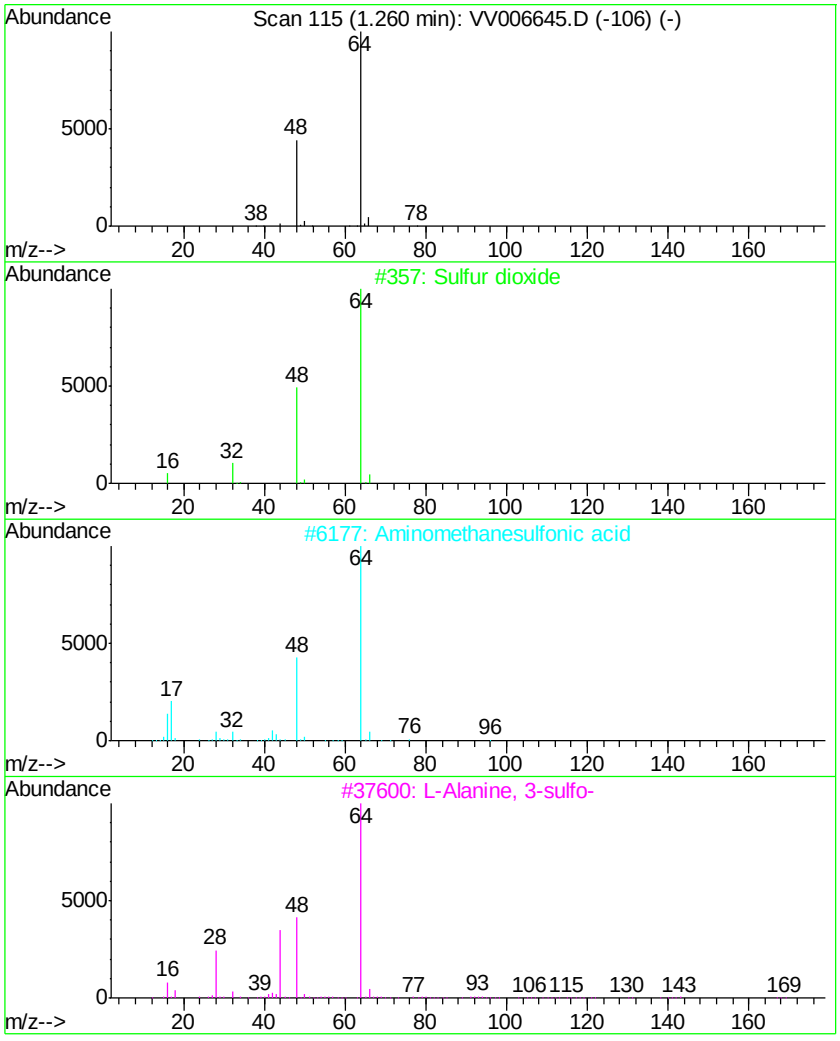
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

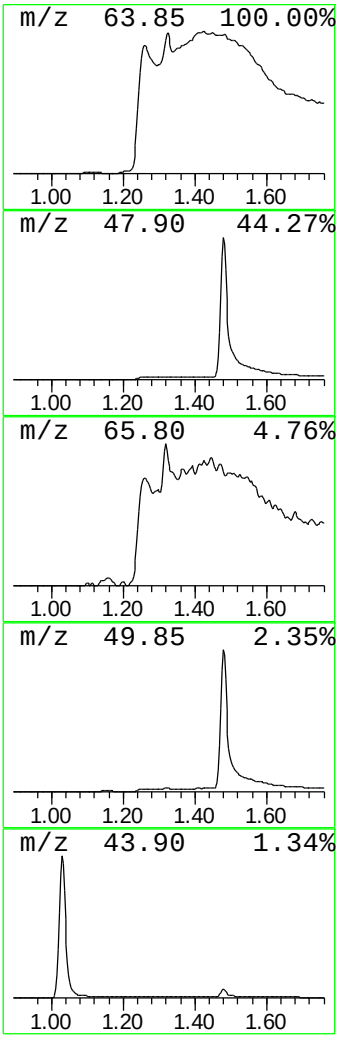
****

Peak Number 2 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	2.36 ug/L	315111	1,4-Difluorobenzene	5.67

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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	5





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV071918\
Data File : VV006645.D
Acq On : 19 Jul 2018 16:21
Operator : SY/MD
Sample : J3983-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

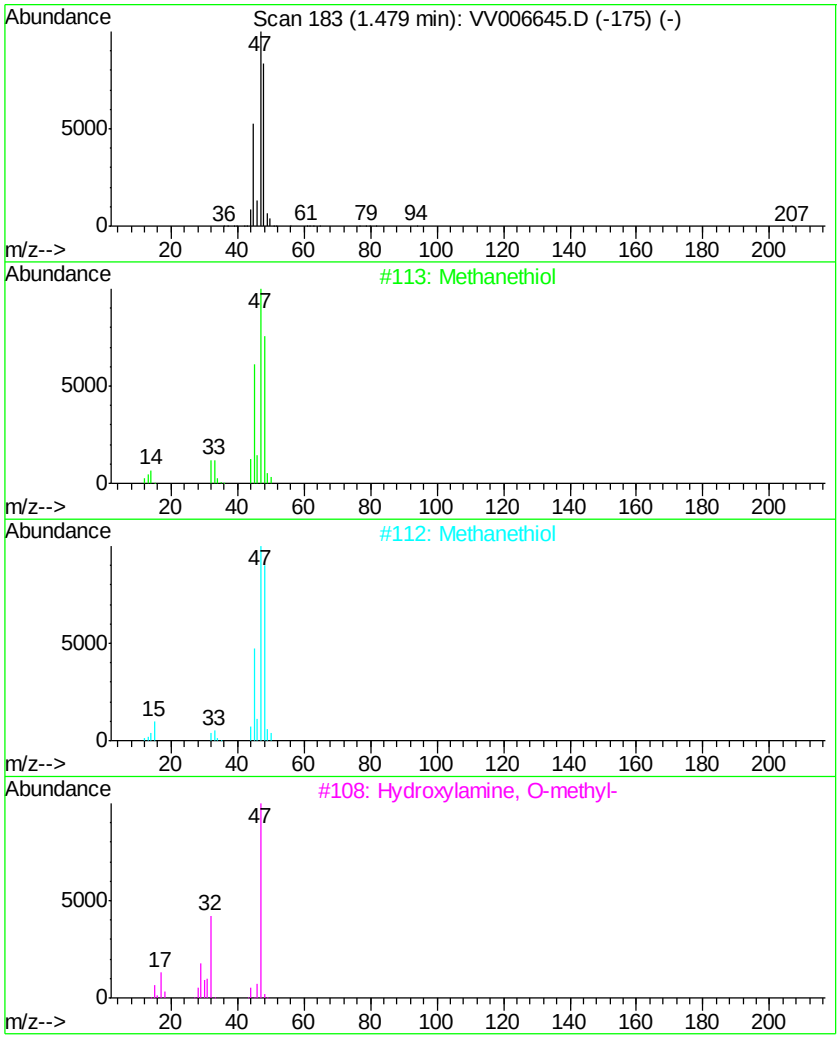
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

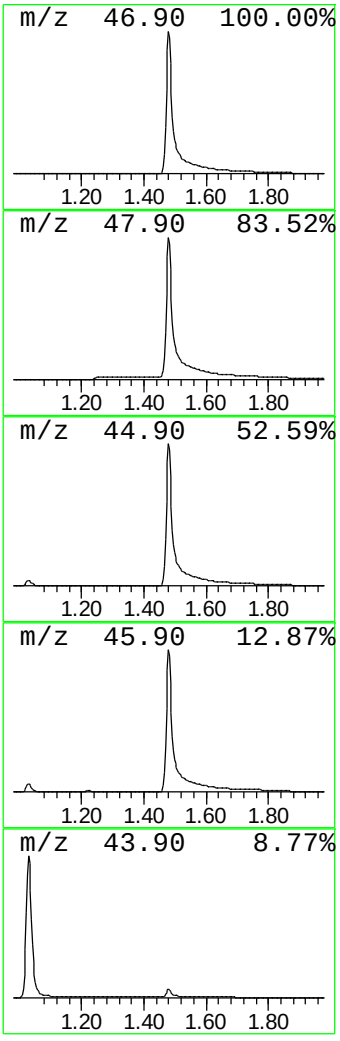
****

Peak Number 3 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	77.40 ug/L	10351300	1,4-Difluorobenzene	5.67

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

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Data File : VV006645.D
Acq On : 19 Jul 2018 16:21
Operator : SY/MD
Sample : J3983-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

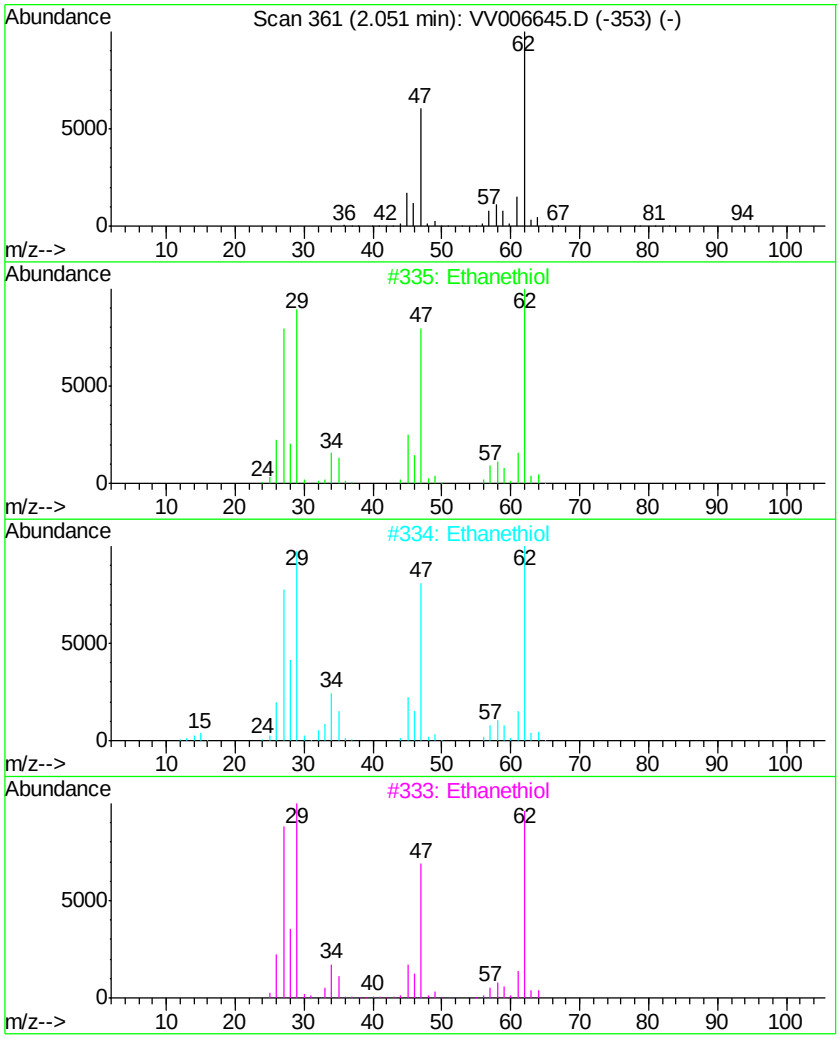
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

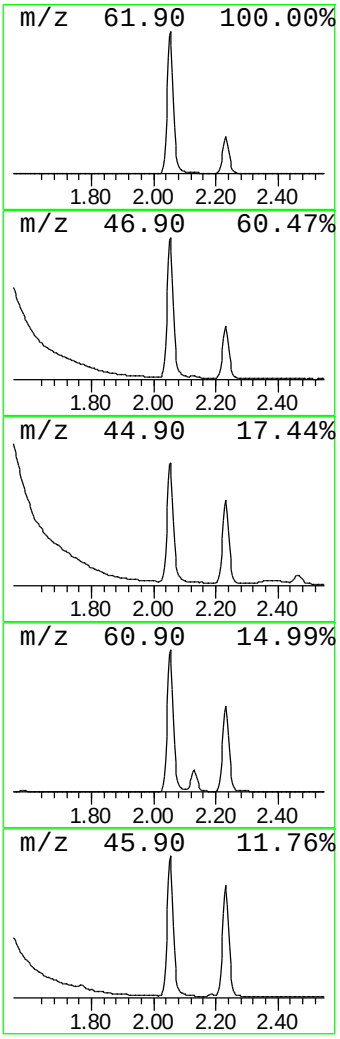
****

Peak Number 4 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	11.40 ug/L	1524710	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol	62	C2H6S	000075-08-1	91
2	Ethanethiol	62	C2H6S	000075-08-1	91
3	Ethanethiol	62	C2H6S	000075-08-1	91
4	Ethanethiol	62	C2H6S	000075-08-1	91
5	Ethanethiol	62	C2H6S	000075-08-1	91





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV071918\
Data File : VV006645.D
Acq On : 19 Jul 2018 16:21
Operator : SY/MD
Sample : J3983-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

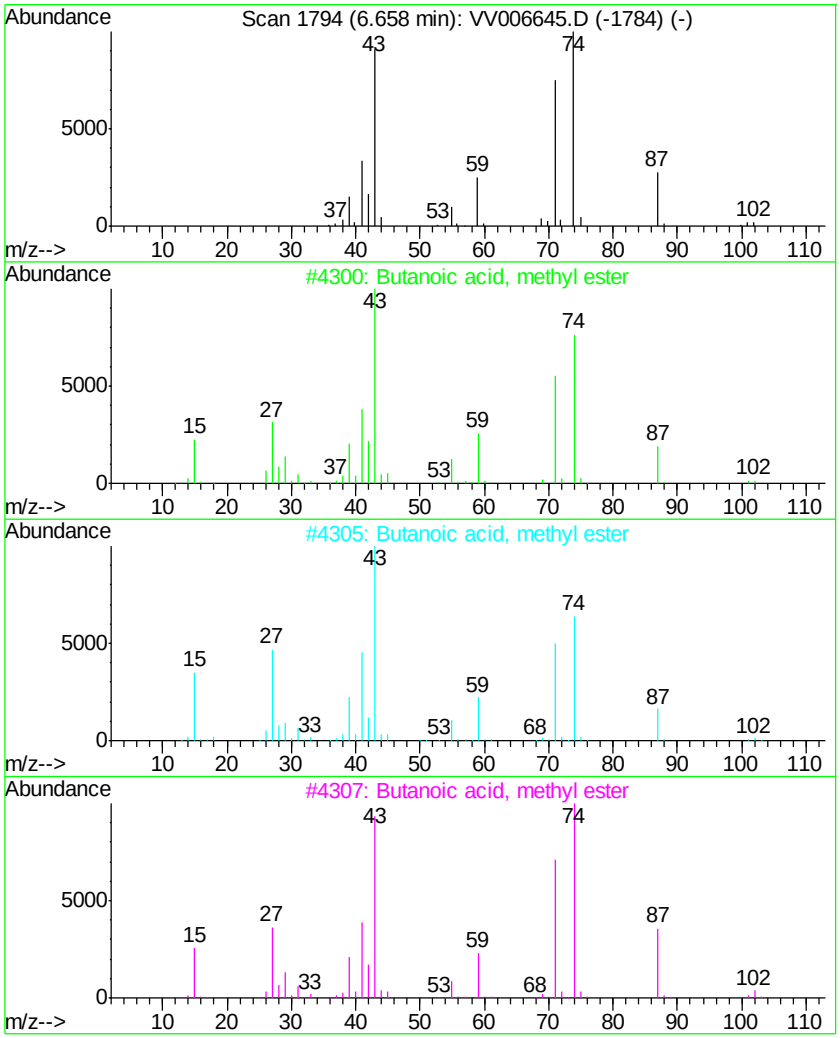
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

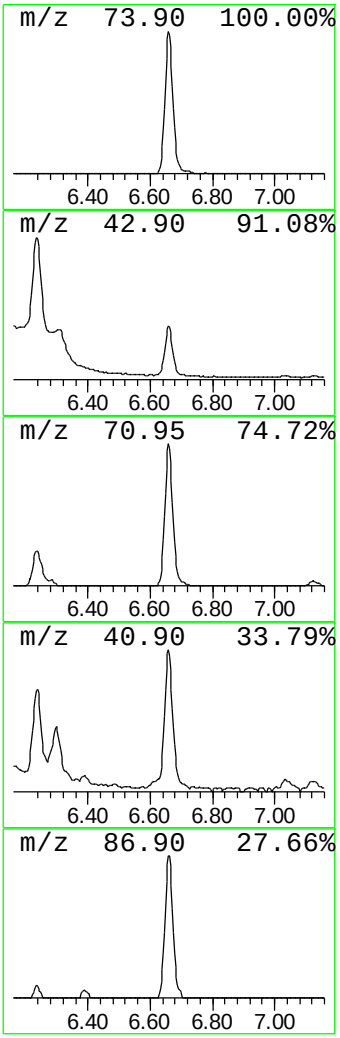
****

Peak Number 5 Butanoic acid, methyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	0.87 ug/L	116750	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
4	2,3,4-Trimethylpentanoic acid	144	C8H16O2	090435-18-0	59
5	Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV071918\
Data File : VV006645.D
Acq On : 19 Jul 2018 16:21
Operator : SY/MD
Sample : J3983-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

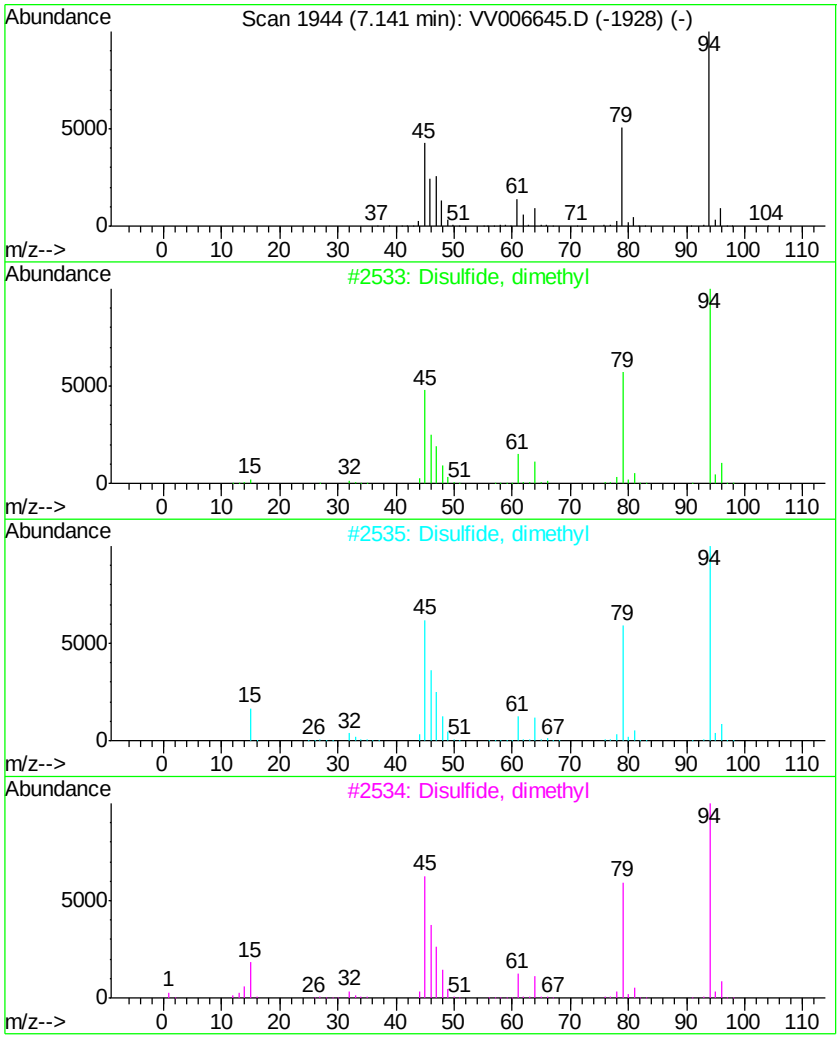
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

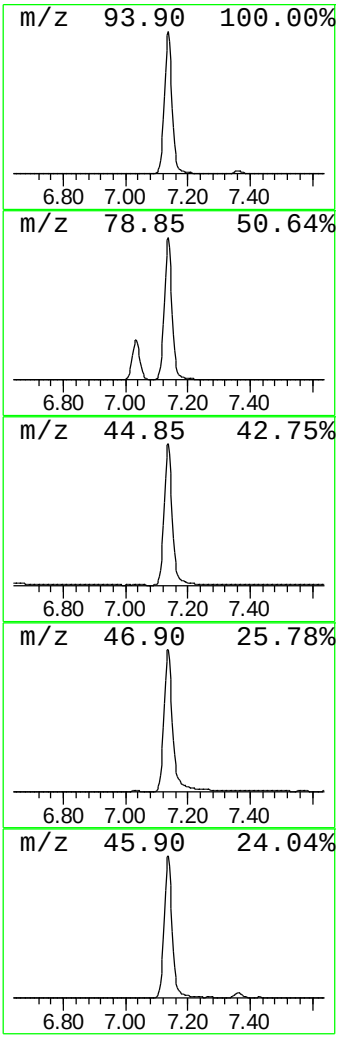
****

Peak Number 7 Disulfide, dimethyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	10.68 ug/L	1428580	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
4	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91





Library Search Compound Report

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Operator : SY/MD
Sample : J3983-19
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

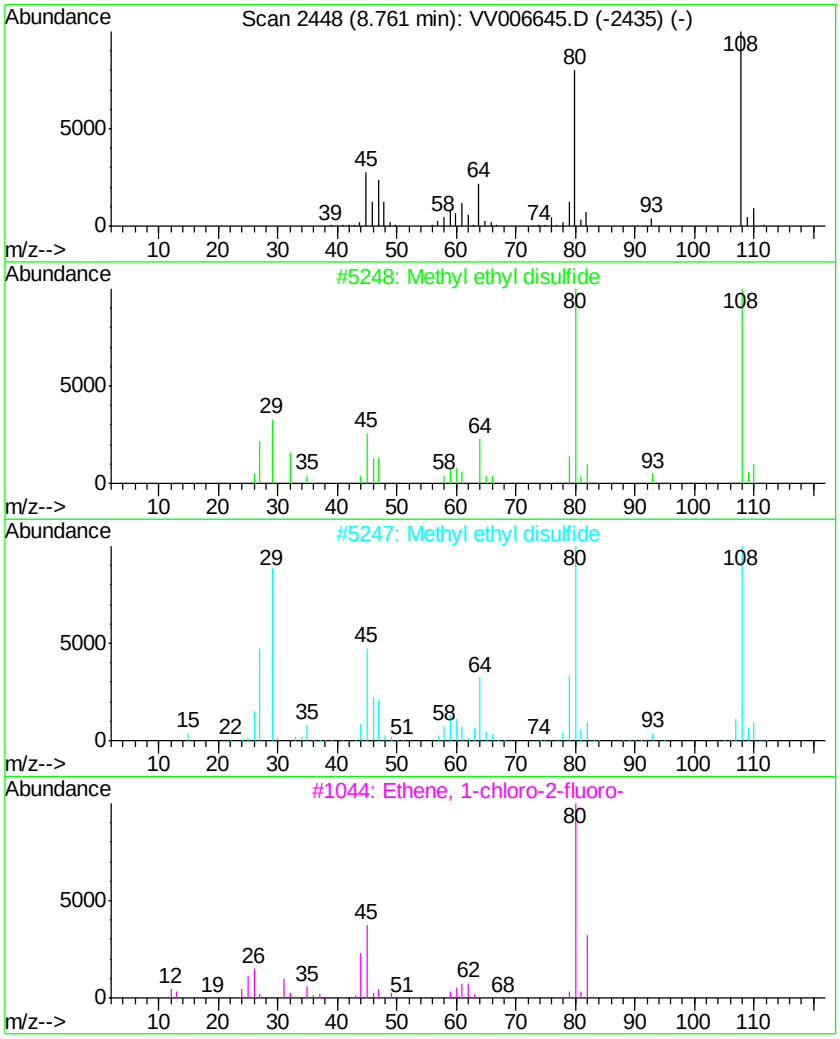
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

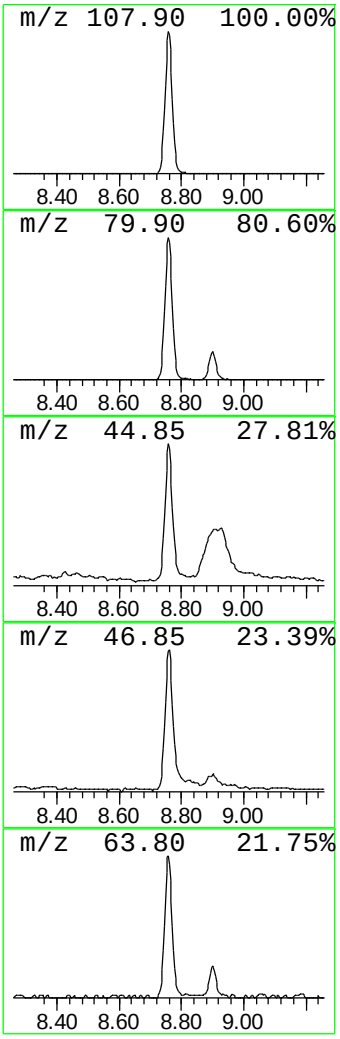
****

Peak Number 8 Methyl ethyl disulfide Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	1.10 ug/L	199570	Chlorobenzene-d5	8.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	86
2	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	72
3	Ethene, 1-chloro-2-fluoro-	80	C2H2ClF	000460-16-2	53
4	Dimethyl phosphite	110	C2H7O3P	000868-85-9	53
5	Methanesulfonic acid, methyl ester	110	C2H6O3S	000066-27-3	53





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Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

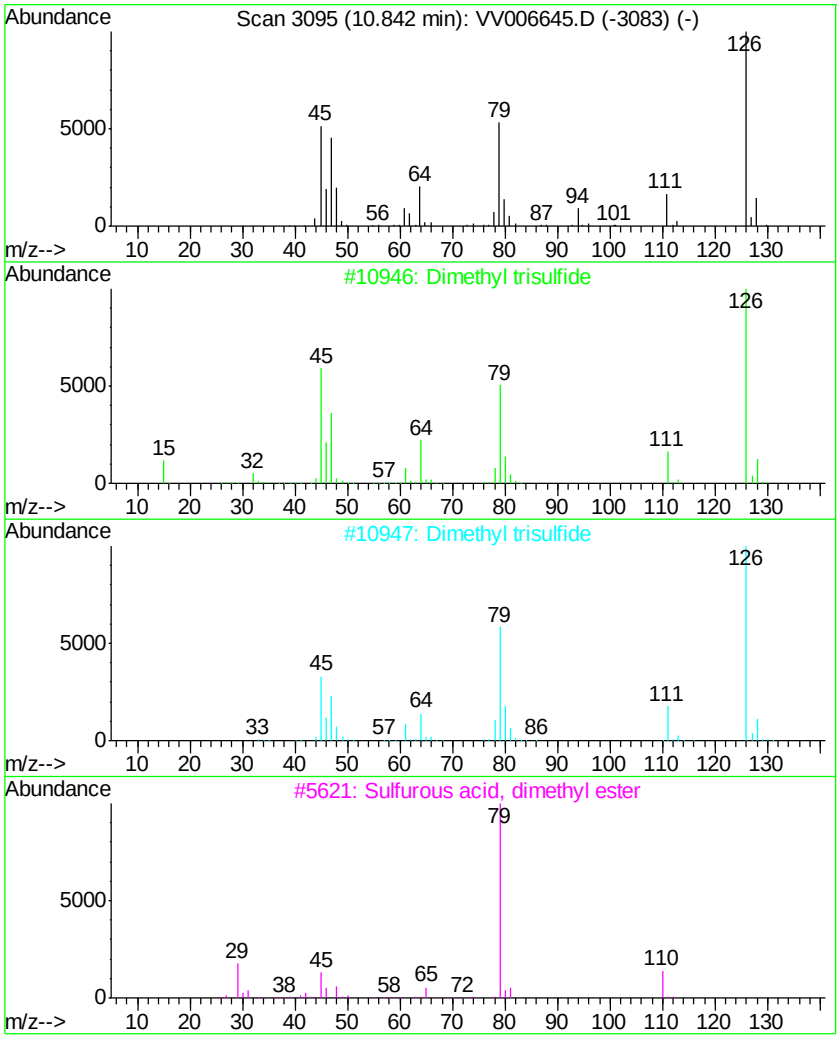
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

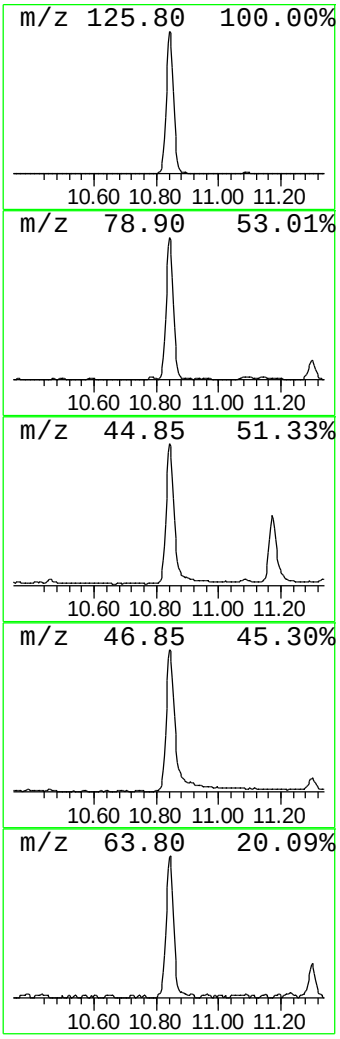
****

Peak Number 9 Dimethyl trisulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	1.58 ug/L	211952	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl trisulfide	126	C2H6S3	003658-80-8	95
2	Dimethyl trisulfide	126	C2H6S3	003658-80-8	93
3	Sulfurous acid, dimethyl ester	110	C2H6O3S	000616-42-2	27
4	1H-Pyrazole-4-carboxamide, 3-amino-	126	C4H6N4O	005334-31-6	14
5	Dimethyldithiophosphinic acid	126	C2H7PS2	016367-68-3	14





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ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

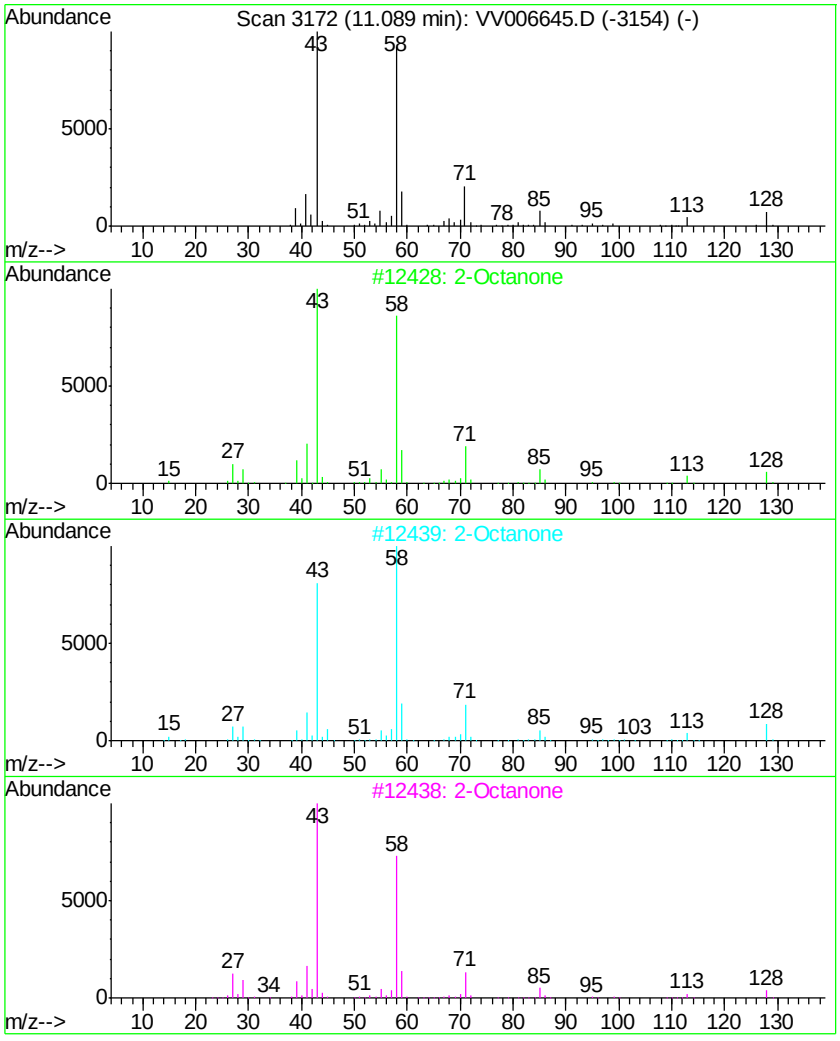
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

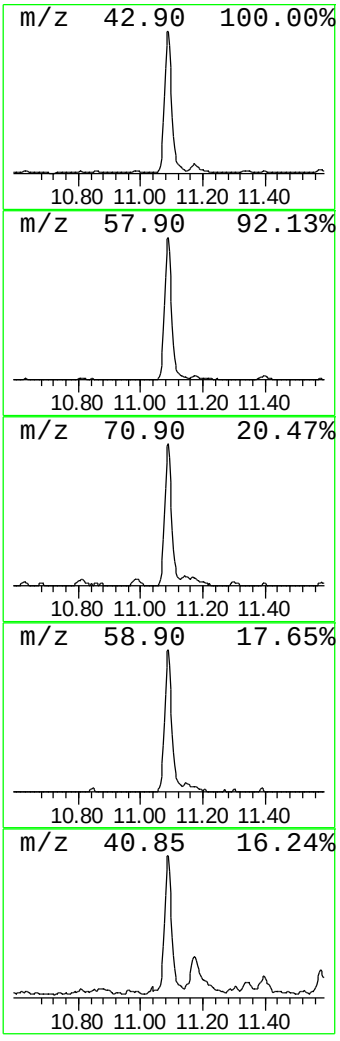
****

Peak Number 10 2-Octanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.09	1.45 ug/L	194845	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	91
2	2-Octanone	128	C8H16O	000111-13-7	91
3	2-Octanone	128	C8H16O	000111-13-7	91
4	2-Octanone	128	C8H16O	000111-13-7	91
5	2-Octanone	128	C8H16O	000111-13-7	91





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ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : DB199

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.M
Quant Title : TRACE VOA SOM01.0

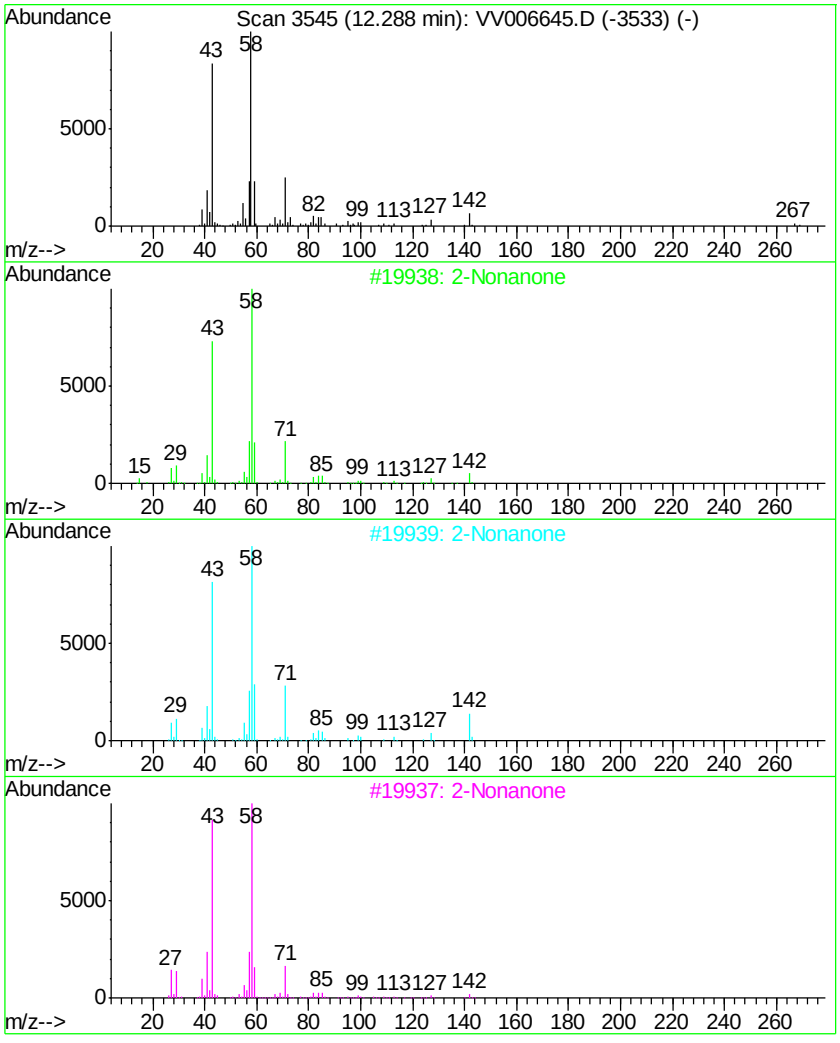
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

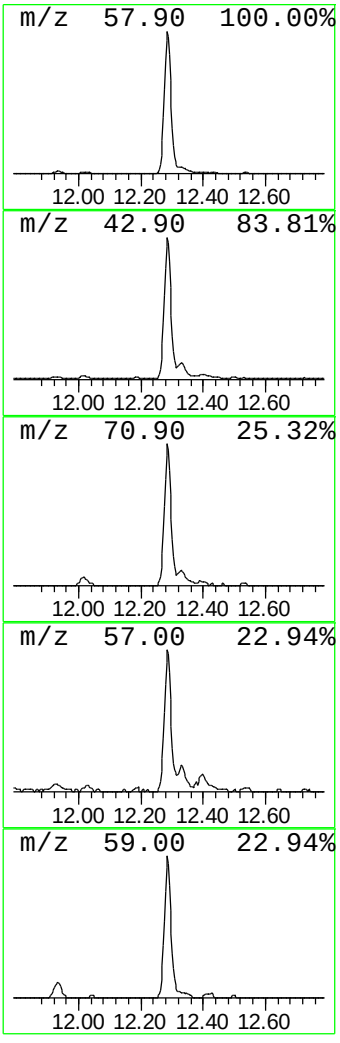
****

Peak Number 11 2-Nonanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	1.36 ug/L	182445	1,4-Dichlorobenzene-d4	11.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone	142	C9H18O	000821-55-6	95
2	2-Nonanone	142	C9H18O	000821-55-6	91
3	2-Nonanone	142	C9H18O	000821-55-6	83
4	2-Dodecanone	184	C12H24O	006175-49-1	78
5	2-Decanone	156	C10H20O	000693-54-9	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV071918\
Data File : VV006645.D
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ALS Vial : 10 Sample Multiplier: 1

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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR071918WMA.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
Sulfur dioxide	1.26	2.4	ug/L	315111	1	5.67	668685	5.0
Methanethiol	1.48	77.4	ug/L	10351300	1	5.67	668685	5.0
Ethanethiol	2.05	11.4	ug/L	1524710	1	5.67	668685	5.0
Butanoic acid, me...	6.66	0.9	ug/L	116750	1	5.67	668685	5.0
Disulfide, dimethyl	7.14	10.7	ug/L	1428580	1	5.67	668685	5.0
Methyl ethyl disu...	8.76	1.1	ug/L	199570	2	8.90	908694	5.0
Dimethyl trisulfide	10.84	1.6	ug/L	211952	3	11.30	672371	5.0
2-Octanone	11.09	1.5	ug/L	194845	3	11.30	672371	5.0
2-Nonanone	12.29	1.4	ug/L	182445	3	11.30	672371	5.0