LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV072018\
Data File : VV006670.D
Acq On : 20 Jul 2018 16:27
Operator : SY/MD
Sample : J4078-02
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AA3

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	1.029	27	43	59	rBV	1092824	1399169	86.86%	12.282%
2	1.093	59	63	73	rVB	22166	30361	1.88%	0.267%
3	1.202	89	97	123	rBV	728247	1610910	100.00%	14.140%
4	1.318	129	133	152	rVB3	151659	207016	12.85%	1.817%
5	1.469	174	180	189	rVB	822256	709286	44.03%	6.226%
6	1.575	208	213	253	rVB	113103	229388	14.24%	2.014%
7	2.054	354	362	375	rVB	125015	172845	10.73%	1.517%
8	2.131	377	386	397	rVB	211888	295327	18.33%	2.592%
9	2.193	398	405	410	rBV	24563	32439	2.01%	0.285%
10	2.231	410	417	433	rVB	75075	113481	7.04%	0.996%
11	2.315	435	443	452	rBV2	30747	51278	3.18%	0.450%
12	2.463	484	489	497	rBV	22566	34286	2.13%	0.301%
13	3.954	938	953	973	rBV2	101627	283607	17.61%	2.489%
14	4.408	1074	1094	1119	rBV	134607	321824	19.98%	2.825%
15	5.099	1289	1309	1349	rBV2	336465	773398	48.01%	6.789%
16	5.668	1471	1486	1508	rBV	270188	545319	33.85%	4.787%
17	6.125	1613	1628	1650	rVB	185259	366294	22.74%	3.215%
18	7.035	1896	1911	1928	rBV	87339	152311	9.45%	1.337%
19	7.138	1929	1943	1978	rBV	231909	434757	26.99%	3.816%
20	7.363	1999	2013	2029	rBV	402868	682472	42.37%	5.991%
21	7.668	2097	2108	2123	rVB	52903	86753	5.39%	0.762%
22	8.141	2242	2255	2284	rBV	432811	724931	45.00%	6.363%
23	8.758	2436	2447	2467	rBV2	48974	82512	5.12%	0.724%
24	8.900	2479	2491	2520	rBV	389535	643550	39.95%	5.649%
25	10.266	2906	2916	2933	rVB	133731	205488	12.76%	1.804%
26	10.842	3083	3095	3109	rBV2	31691	54110	3.36%	0.475%
27	11.089	3157	3172	3182	rBV2	11682	19589	1.22%	0.172%
28	11.301	3225	3238	3260	rBV	364087	574706	35.68%	5.045%
29	11.678	3343	3355	3376	rVB	339118	534968	33.21%	4.696%
30	12.289	3533	3545	3556	rBV4	10457	19956	1.24%	0.175%

Sum of corrected areas: 11392331

LSC Report - Integrated Chromatogram

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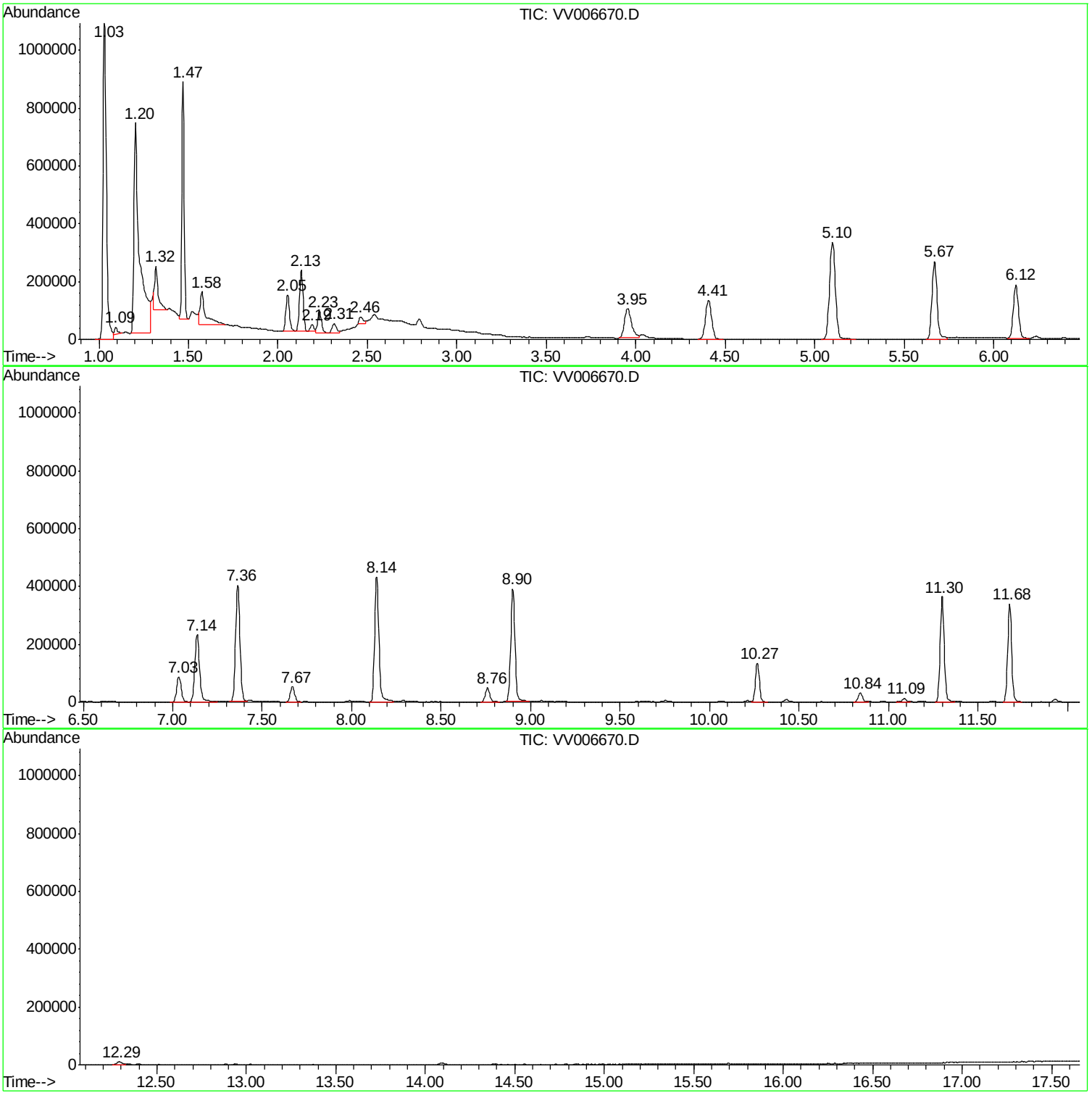
Sample : J4078-02
Misc : 25 mL/MSVOA V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AA3

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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Quant Title : TRACE VOA SOM01.0

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

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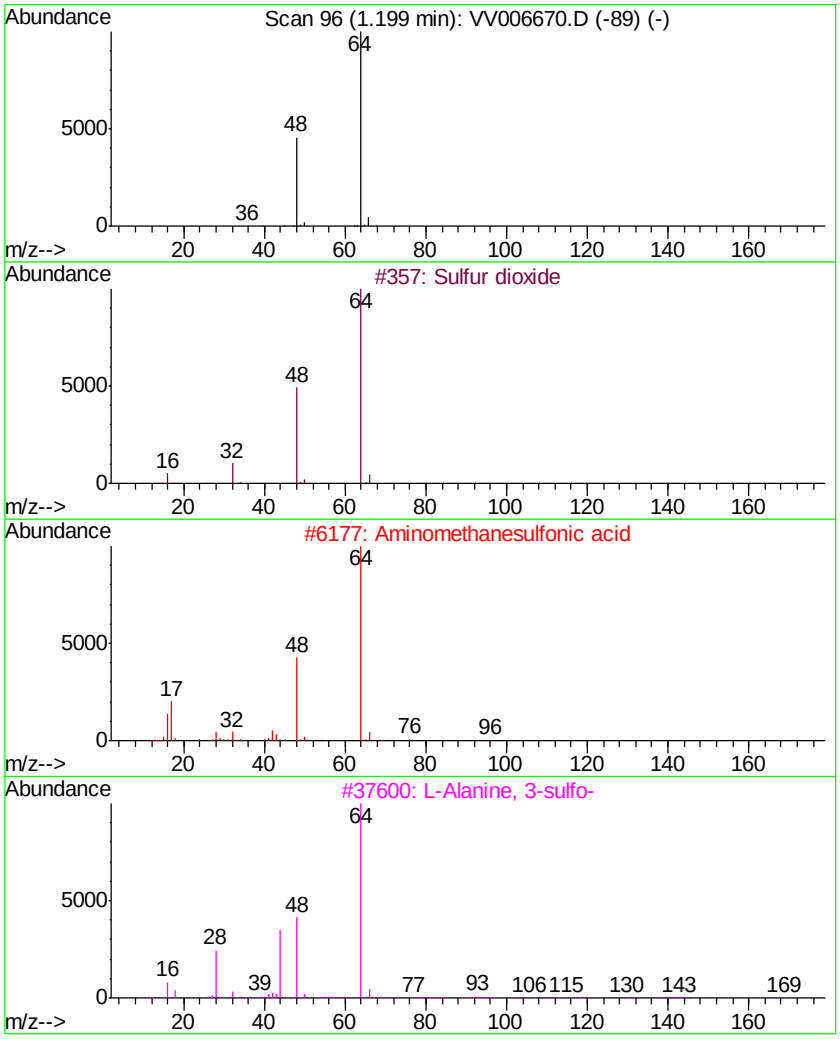
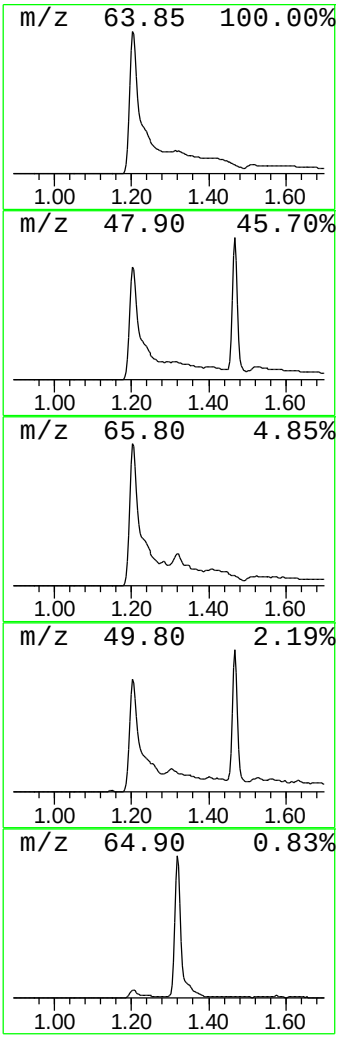
Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.20	14.77 ug/L	1610910	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	Sulfur dioxide	64	O2S	007446-09-5	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





Library Search Compound Report

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Operator : SY/MD
Sample : J4078-02
Misc : 25 mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AA3

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

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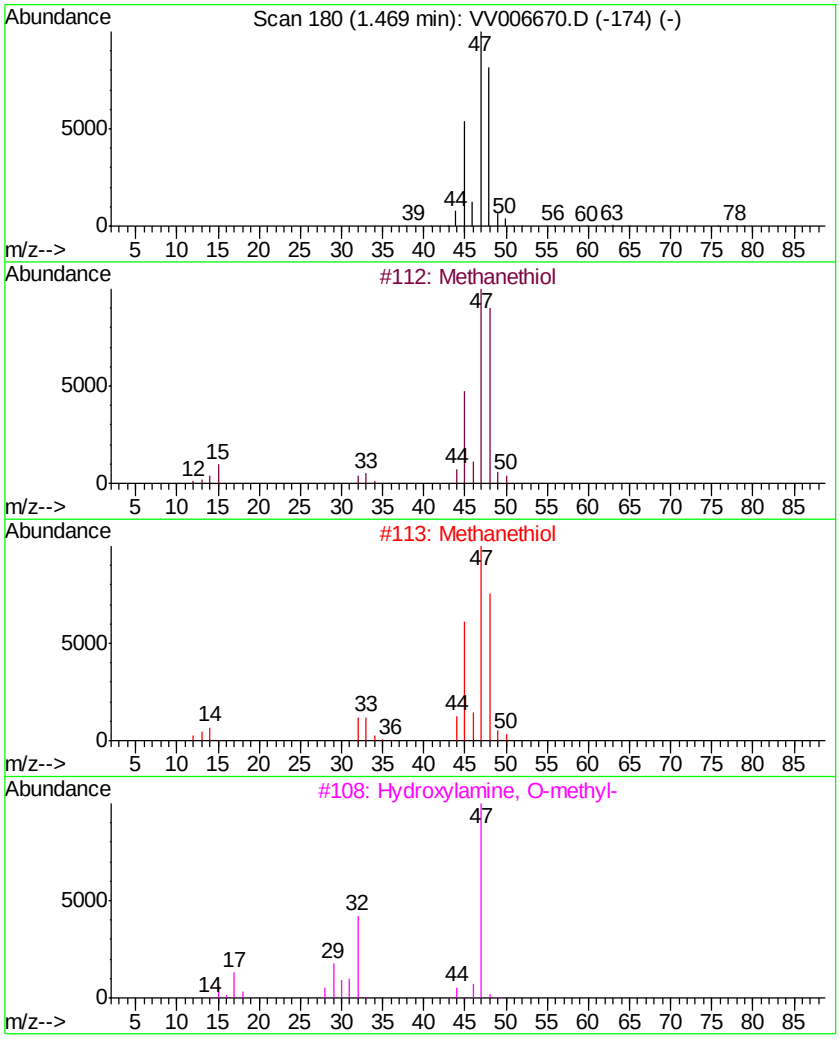
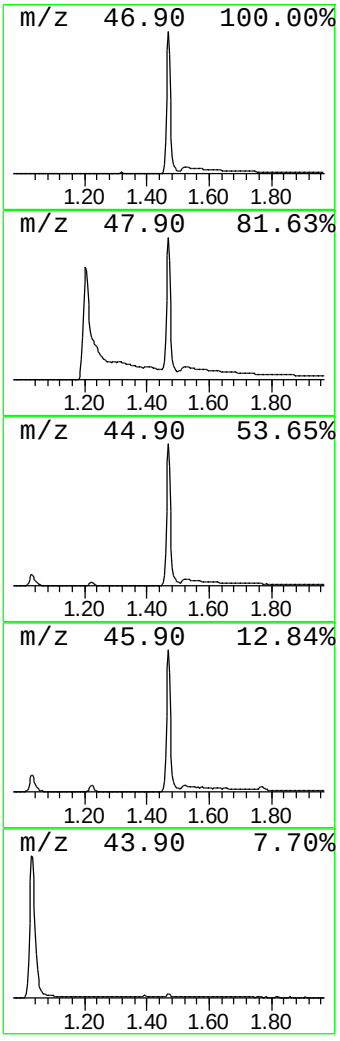
Peak Number 3 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	6.50 ug/L	709286	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	83
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





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Instrument : MSVOA_V
ClientSampleId : C0AA3

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

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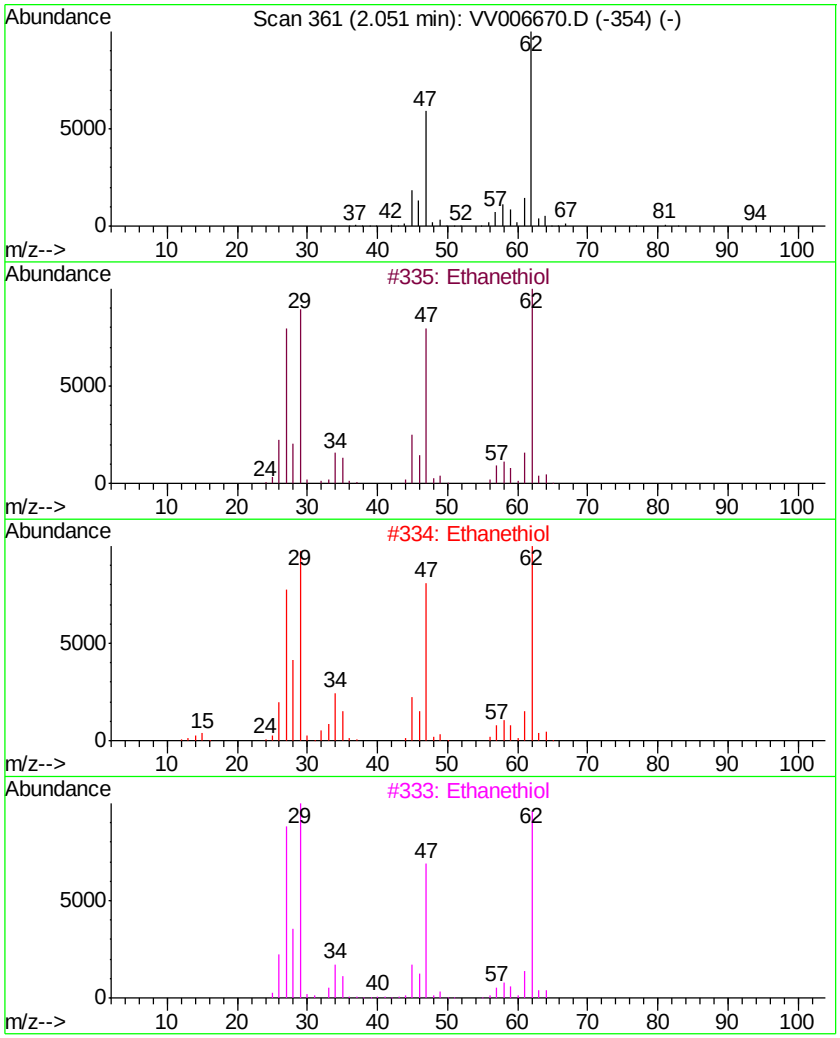
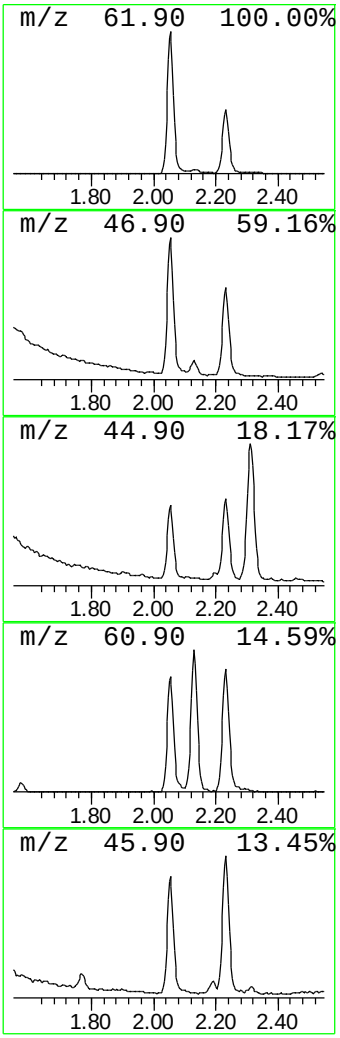
Peak Number 4 Ethanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	1.58 ug/L	172845	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





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Instrument : MSVOA_V
ClientSampleId : C0AA3

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

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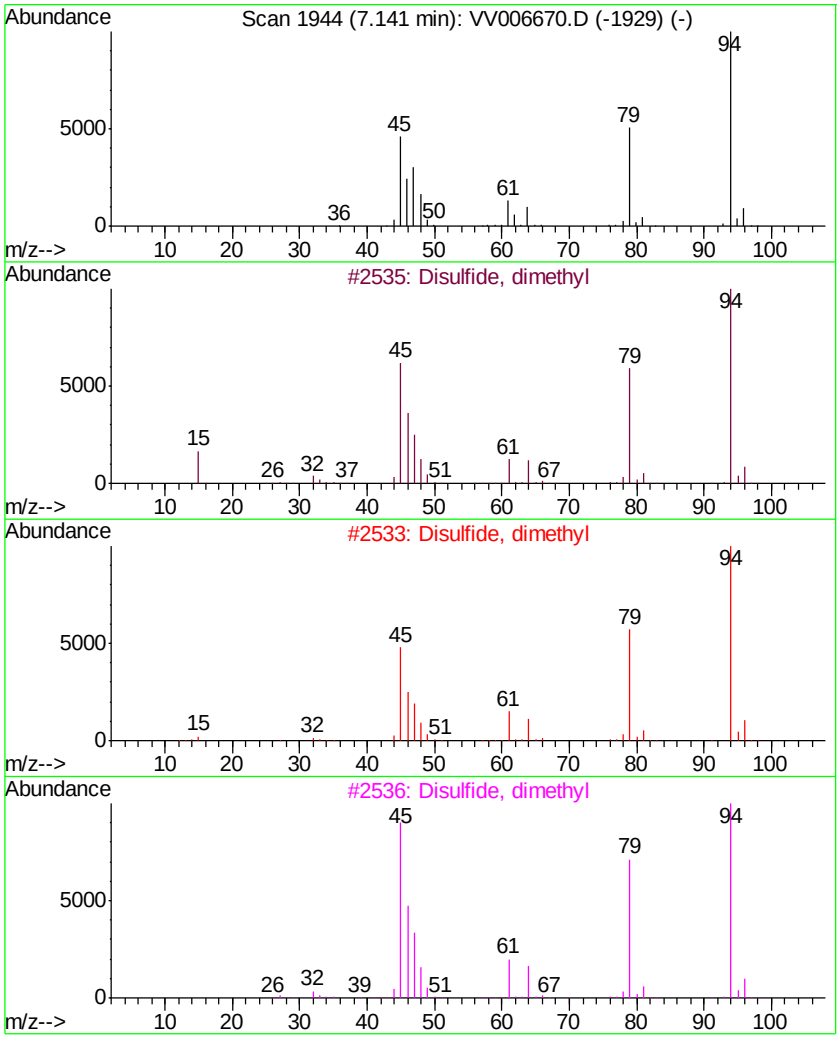
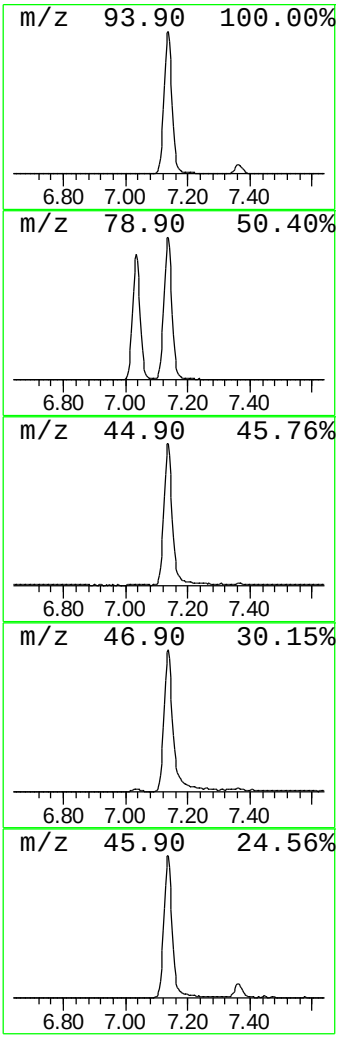
Peak Number 6 Disulfide, dimethyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.14	3.99 ug/L	434757	1,4-Difluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
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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ALS Vial : 15 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AA3

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

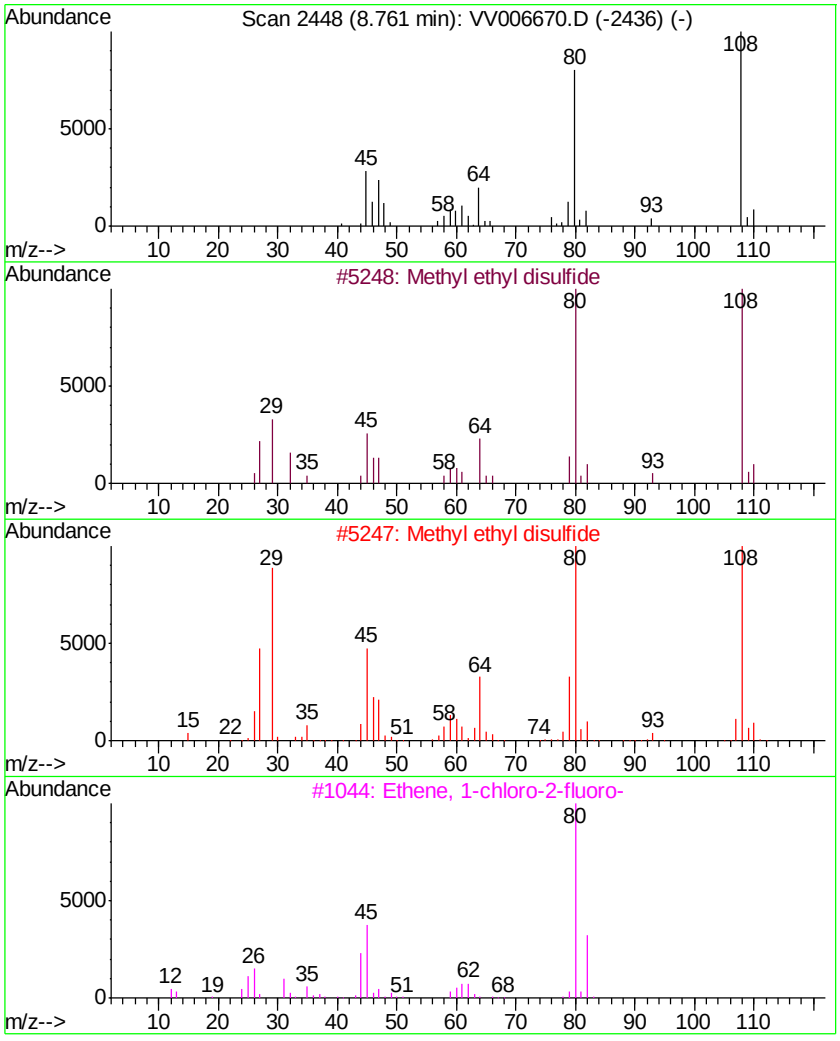
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

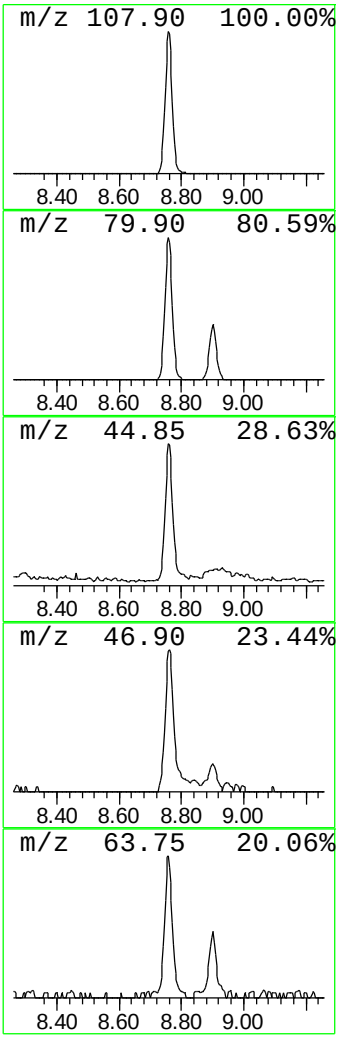
****

Peak Number 7 Methyl ethyl disulfide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.76	0.64 ug/L	82512	Chlorobenzene-d5	8.90

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	87
2	Methyl ethyl disulfide	108	C3H8S2	020333-39-5	78
3	Ethene, 1-chloro-2-fluoro-	80	C2H2ClF	000460-16-2	53
4	Dimethyl phosphite	110	C2H7O3P	000868-85-9	50
5	Dimethyl phosphite	110	C2H7O3P	000868-85-9	50





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	1.20	14.8	ug/L	1610910	1	5.67	545319	5.0
Methanethiol	1.47	6.5	ug/L	709286	1	5.67	545319	5.0
Ethanethiol	2.05	1.6	ug/L	172845	1	5.67	545319	5.0
Disulfide, dimethyl	7.14	4.0	ug/L	434757	1	5.67	545319	5.0
Methyl ethyl disu...	8.76	0.6	ug/L	82512	2	8.90	643550	5.0