LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061622\
Data File : VU049231.D
Acq On : 17 Jun 2022 01:54
Operator : SY/MD
Sample : N3320-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGJ93

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_U\Method\SFAMUTR061422WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU049231.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.498	41	49	63	rBV	51374	152083	6.14%	1.344%
2	1.604	74	82	104	rVB	487791	573229	23.15%	5.066%
3	1.790	134	140	154	rVB	28728	37610	1.52%	0.332%
4	1.912	172	178	190	rVB	42299	57284	2.31%	0.506%
5	2.472	342	352	363	rVB2	17906	28160	1.14%	0.249%
6	2.581	370	386	395	rBV	661138	1120181	45.25%	9.901%
7	2.639	395	404	439	rVB	316914	753415	30.43%	6.659%
8	2.954	490	502	522	rBV	146922	284611	11.50%	2.516%
9	3.871	769	787	819	rBV	289645	691853	27.95%	6.115%
10	4.436	948	963	986	rBV	97531	236766	9.56%	2.093%
11	4.668	1010	1035	1076	rBV3	859012	2475624	100.00%	21.881%
12	5.063	1133	1158	1180	rBV	84554	191392	7.73%	1.692%
13	5.198	1187	1200	1218	rBV	55086	116031	4.69%	1.026%
14	5.726	1343	1364	1380	rBV2	155770	413942	16.72%	3.659%
15	6.250	1514	1527	1551	rBV	133288	250666	10.13%	2.216%
16	6.542	1597	1618	1649	rBV	825311	1553835	62.77%	13.734%
17	6.690	1651	1664	1680	rVV	103236	203914	8.24%	1.802%
18	6.780	1681	1692	1712	rVB4	27548	69493	2.81%	0.614%
19	7.568	1924	1937	1951	rBV	45390	81850	3.31%	0.723%
20	7.899	2027	2040	2054	rBV	188102	323759	13.08%	2.862%
21	8.179	2117	2127	2140	rBV2	30221	51305	2.07%	0.453%
22	8.636	2256	2269	2307	rBV	308019	591314	23.89%	5.226%
23	9.417	2499	2512	2528	rBV	181792	302124	12.20%	2.670%
24	10.758	2918	2929	2944	rVB	89252	144368	5.83%	1.276%
25	11.812	3245	3257	3276	rBV	191527	304112	12.28%	2.688%
26	12.192	3363	3375	3395	rBV	186798	305224	12.33%	2.698%

Sum of corrected areas: 11314145

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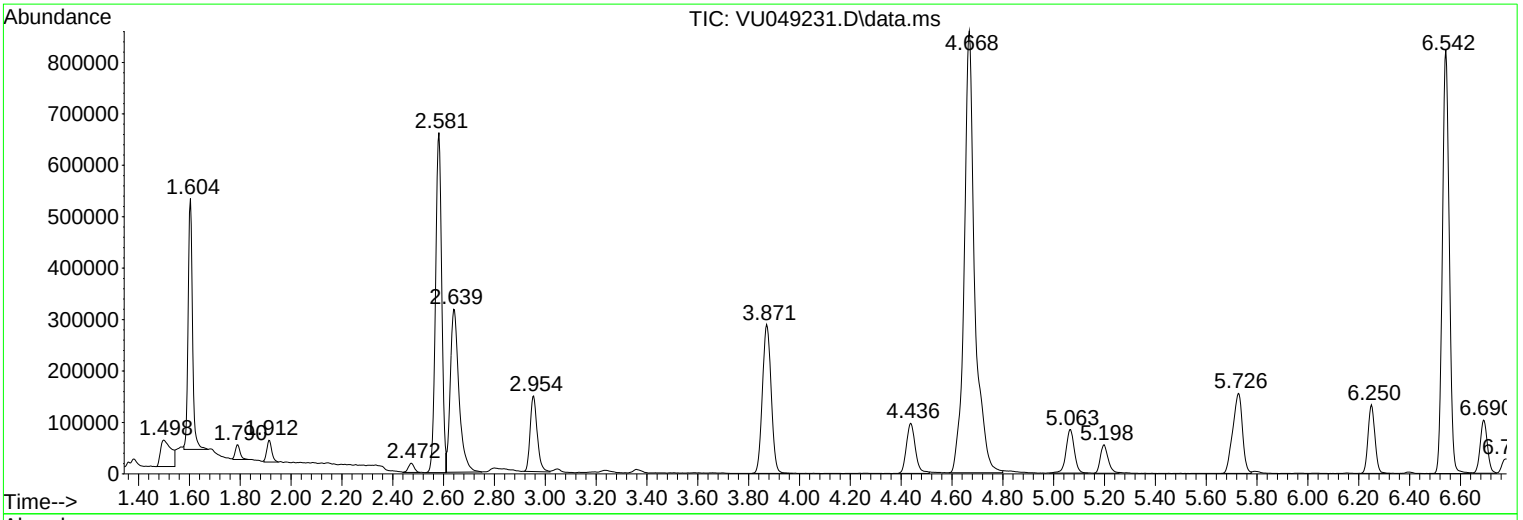
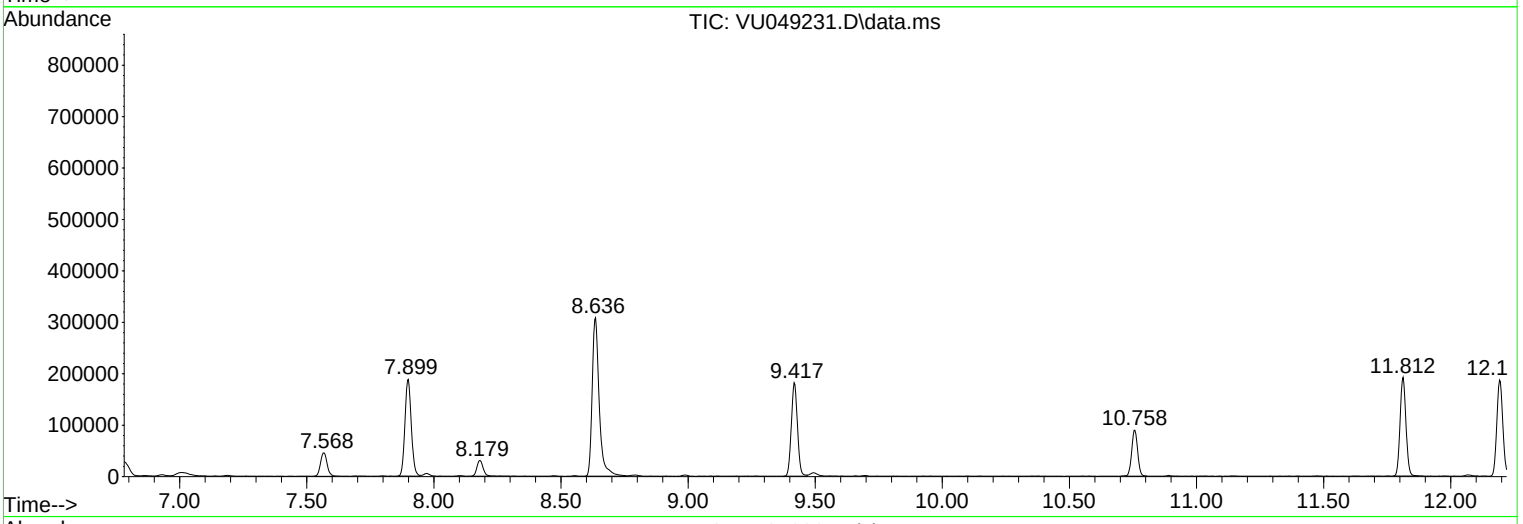
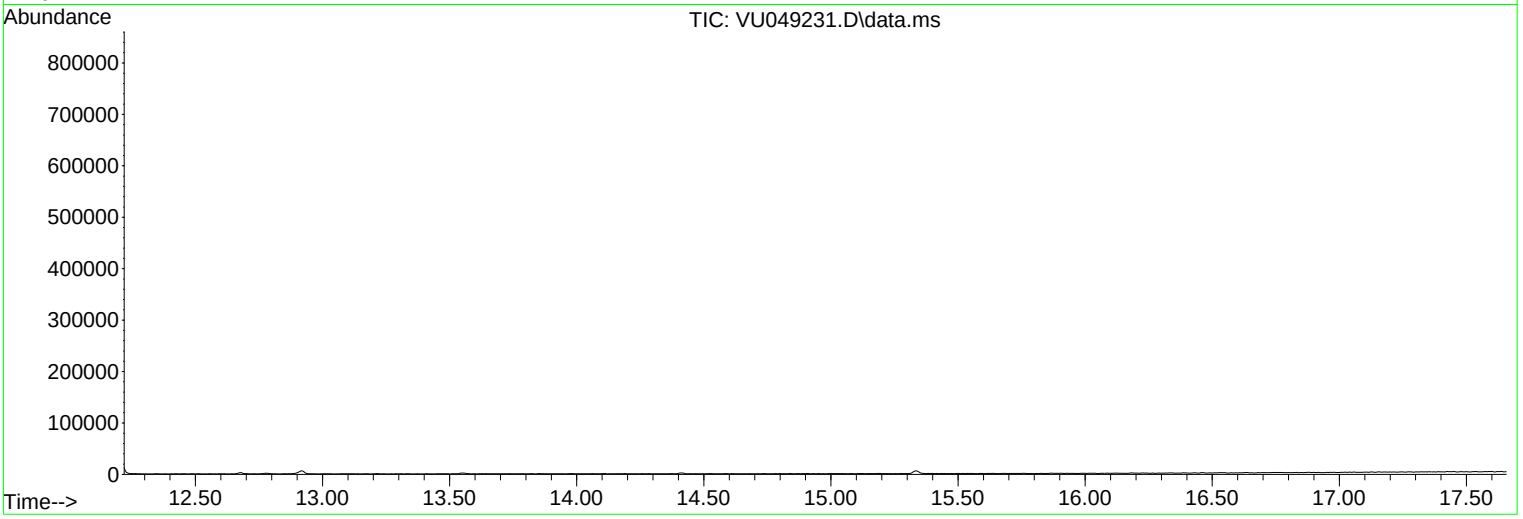
ClientSampleId :
BGJ93

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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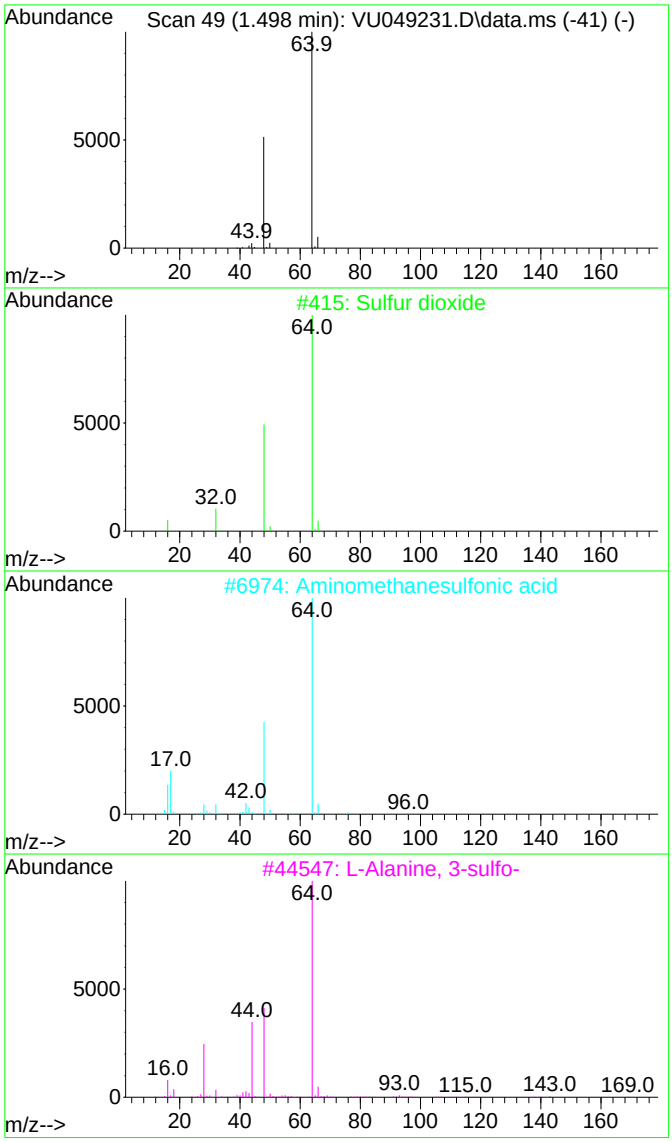
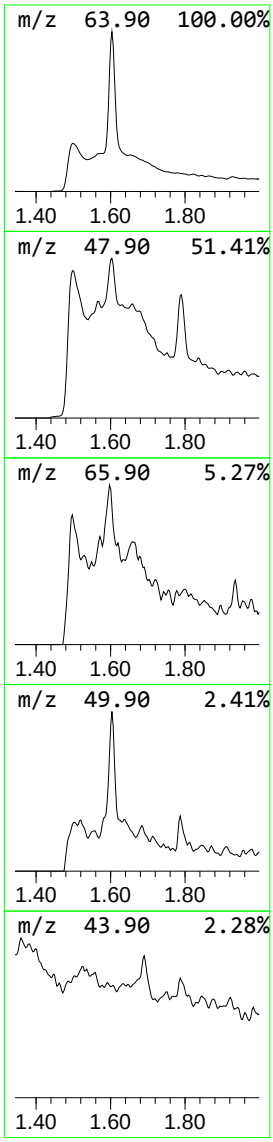
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.498	3.03 ug/L	152083	1,4-Difluorobenzene	6.250

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	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9





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Operator : SY/MD
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGJ93

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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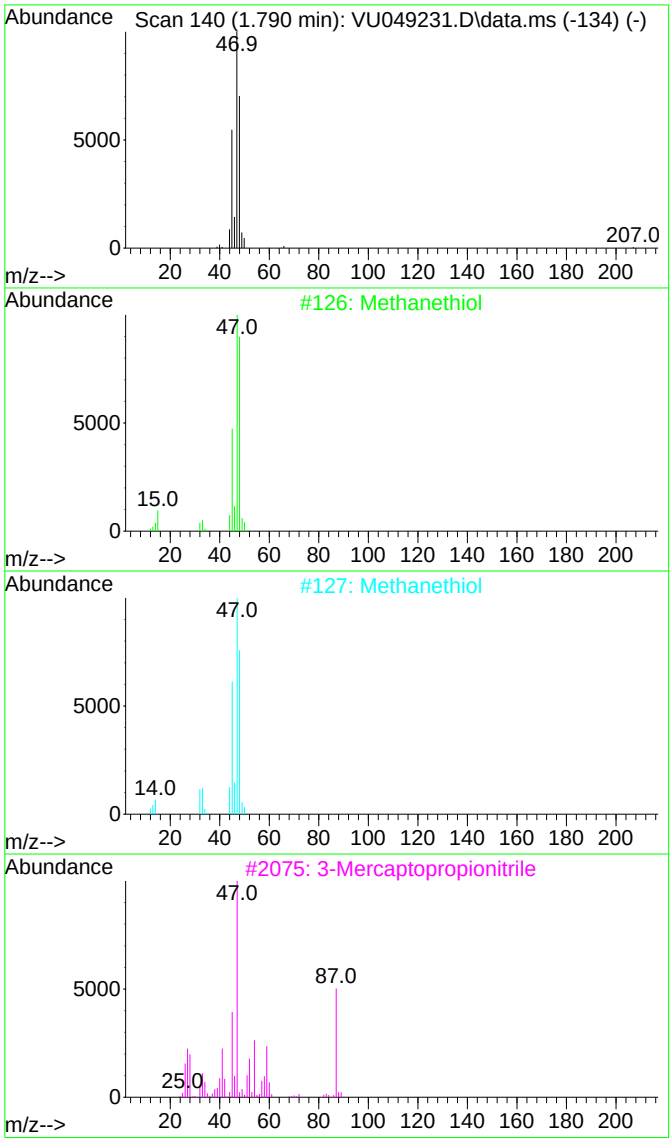
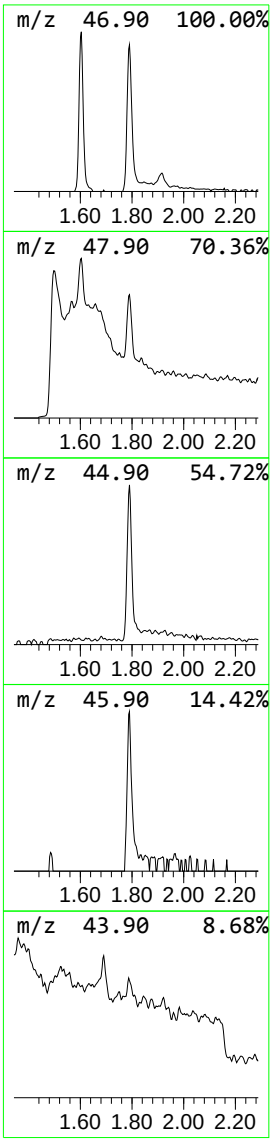
Peak Number 2 Methanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.790	0.75 ug/L	37610	1,4-Difluorobenzene	6.250

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	3-Mercaptopropionitrile	87	C3H5NS	001001-58-7	36
4	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	9
5	Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9





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Operator : SY/MD
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGJ93

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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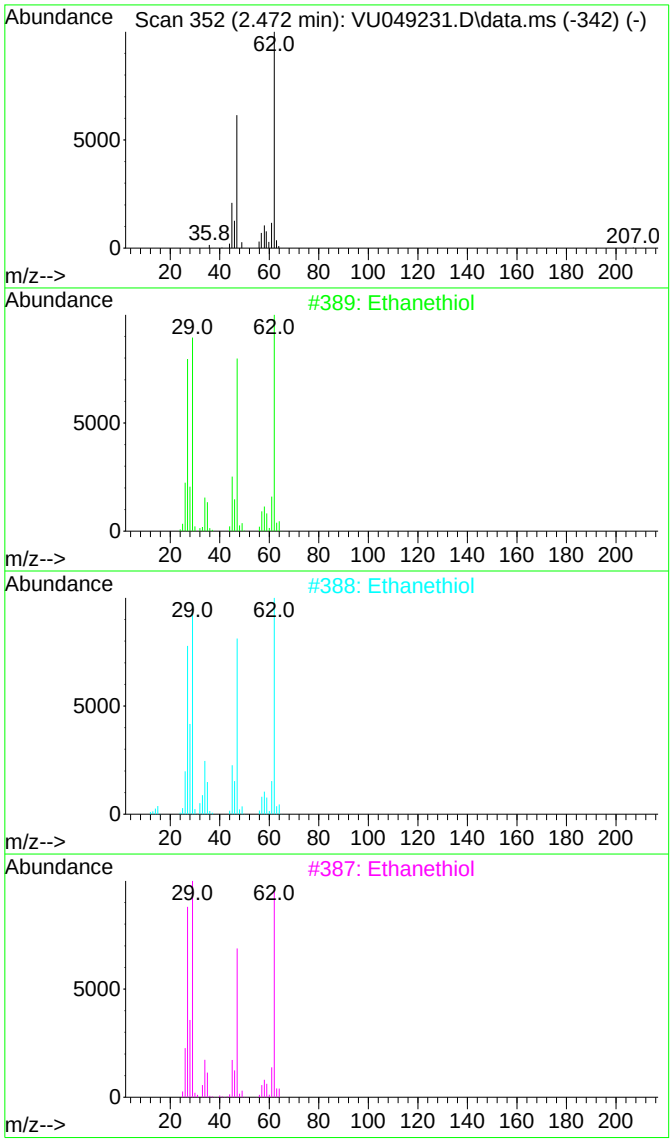
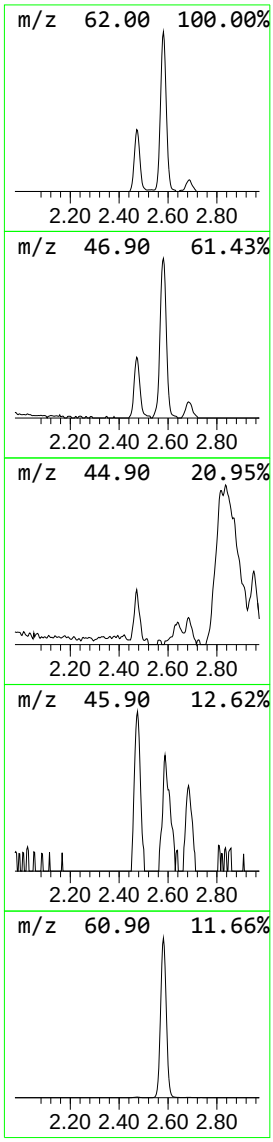
Peak Number 3 Ethanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.472	0.56 ug/L	28160	1,4-Difluorobenzene	6.250

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	90





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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGJ93

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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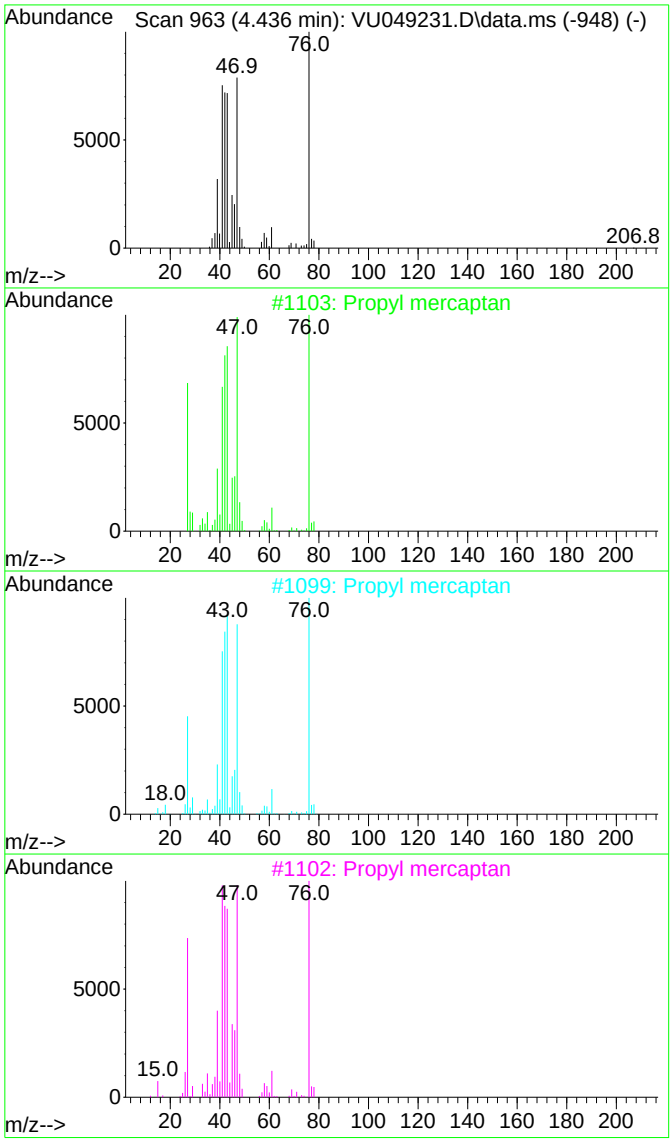
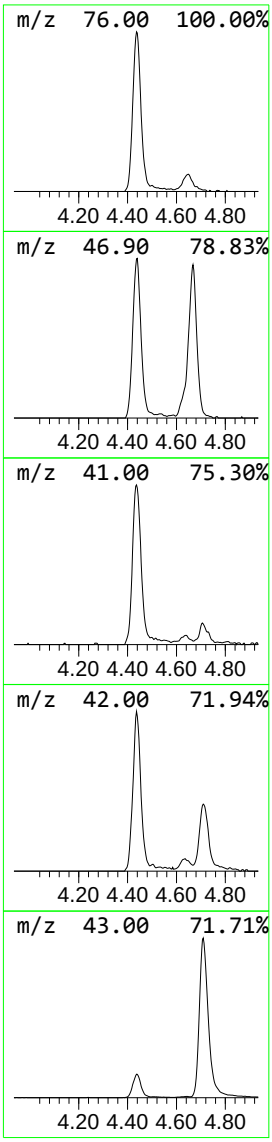
Peak Number 4 Propyl mercaptan Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.436	4.72 ug/L	236766	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	97
2	Propyl mercaptan	76	C3H8S	000107-03-9	95
3	Propyl mercaptan	76	C3H8S	000107-03-9	91
4	Propyl mercaptan	76	C3H8S	000107-03-9	91
5	Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	83





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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGJ93

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061422WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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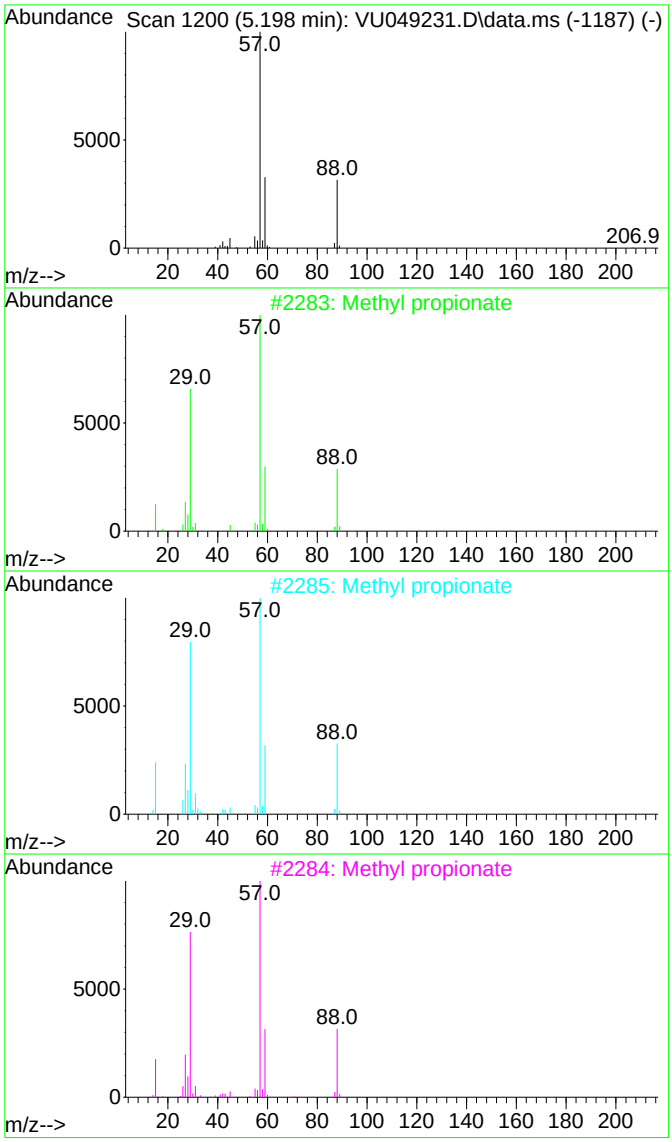
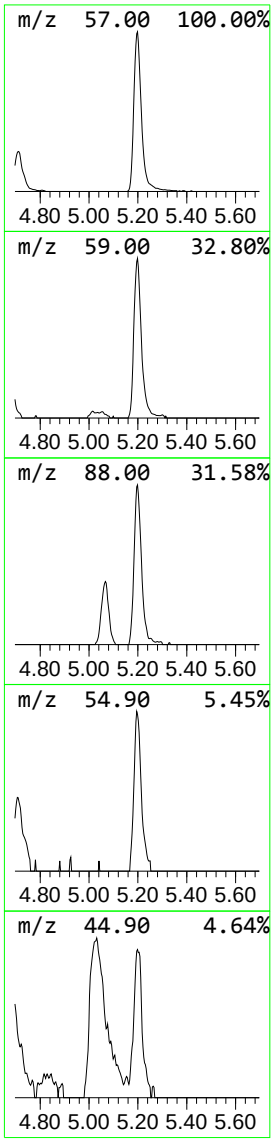
Peak Number 5 Methyl propionate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.198	2.31 ug/L	116031	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl propionate	88	C4H8O2	000554-12-1	90
2	Methyl propionate	88	C4H8O2	000554-12-1	90
3	Methyl propionate	88	C4H8O2	000554-12-1	86
4	Methyl propionate	88	C4H8O2	000554-12-1	58
5	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	9





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.498	3.0	ug/L	152083	1	6.250	250666	5.0
Methanethiol	1.790	0.8	ug/L	37610	1	6.250	250666	5.0
Ethanethiol	2.472	0.6	ug/L	28160	1	6.250	250666	5.0
Propyl mercaptan	4.436	4.7	ug/L	236766	1	6.250	250666	5.0
Methyl propionate	5.198	2.3	ug/L	116031	1	6.250	250666	5.0