LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011224\
Data File : VV033615.D
Acq On : 12 Jan 2024 23:28
Operator : SY/MD
Sample : P1121-07
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

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\SFAMVTR011224WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VV033615.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.098	11	18	24	rBV2	9861	13878	1.77%	0.321%
2	1.169	33	40	57	rVB	91555	118323	15.10%	2.735%
3	1.285	66	76	102	rBV	359065	609099	77.75%	14.080%
4	1.426	116	120	132	rBV	24977	27390	3.50%	0.633%
5	1.986	288	294	306	rVV3	22835	38949	4.97%	0.900%
6	2.072	310	321	329	rVV	348367	545942	69.69%	12.620%
7	2.111	329	333	356	rVB	71315	112897	14.41%	2.610%
8	2.375	402	415	431	rBV	30715	54546	6.96%	1.261%
9	3.114	630	645	671	rBV	118563	251138	32.06%	5.805%
10	3.593	782	794	818	rBV	35834	91759	11.71%	2.121%
11	3.815	846	863	876	rBV3	289919	783365	100.00%	18.108%
12	4.256	986	1000	1019	rBV2	23300	65148	8.32%	1.506%
13	4.963	1206	1220	1247	rBV3	52714	141637	18.08%	3.274%
14	5.542	1390	1400	1421	rBV2	42982	92452	11.80%	2.137%
15	5.834	1479	1491	1524	rBV	192551	394251	50.33%	9.113%
16	5.995	1529	1541	1558	rBV	29683	64813	8.27%	1.498%
17	6.297	1625	1635	1655	rBV4	6981	16555	2.11%	0.383%
18	6.924	1820	1830	1849	rBV3	14097	29799	3.80%	0.689%
19	7.249	1921	1931	1954	rBV	57300	107076	13.67%	2.475%
20	7.567	2019	2030	2050	rBV3	8293	17200	2.20%	0.398%
21	8.027	2164	2173	2210	rBV	153610	316237	40.37%	7.310%
22	8.789	2401	2410	2437	rBV	68463	122364	15.62%	2.829%
23	10.156	2826	2835	2848	rBV2	36620	56466	7.21%	1.305%
24	11.188	3147	3156	3174	rBV	77145	128438	16.40%	2.969%
25	11.509	3247	3256	3263	rBV5	4535	9438	1.20%	0.218%
26	11.564	3263	3273	3292	rVB	70733	116913	14.92%	2.703%

Sum of corrected areas: 4326073

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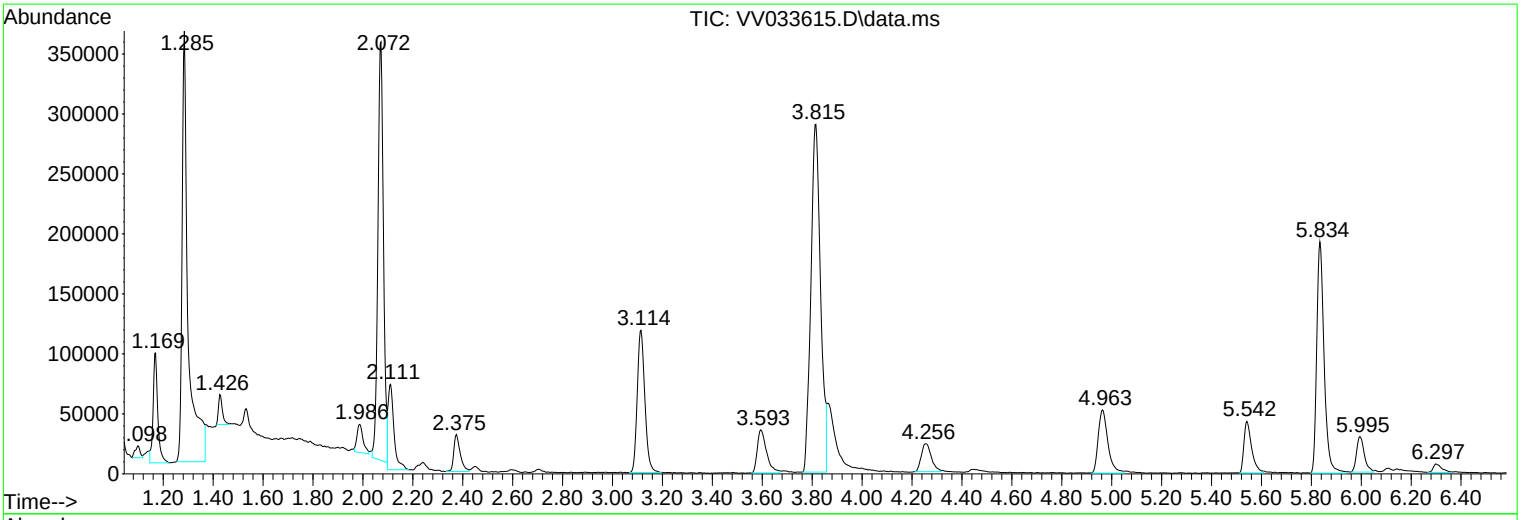
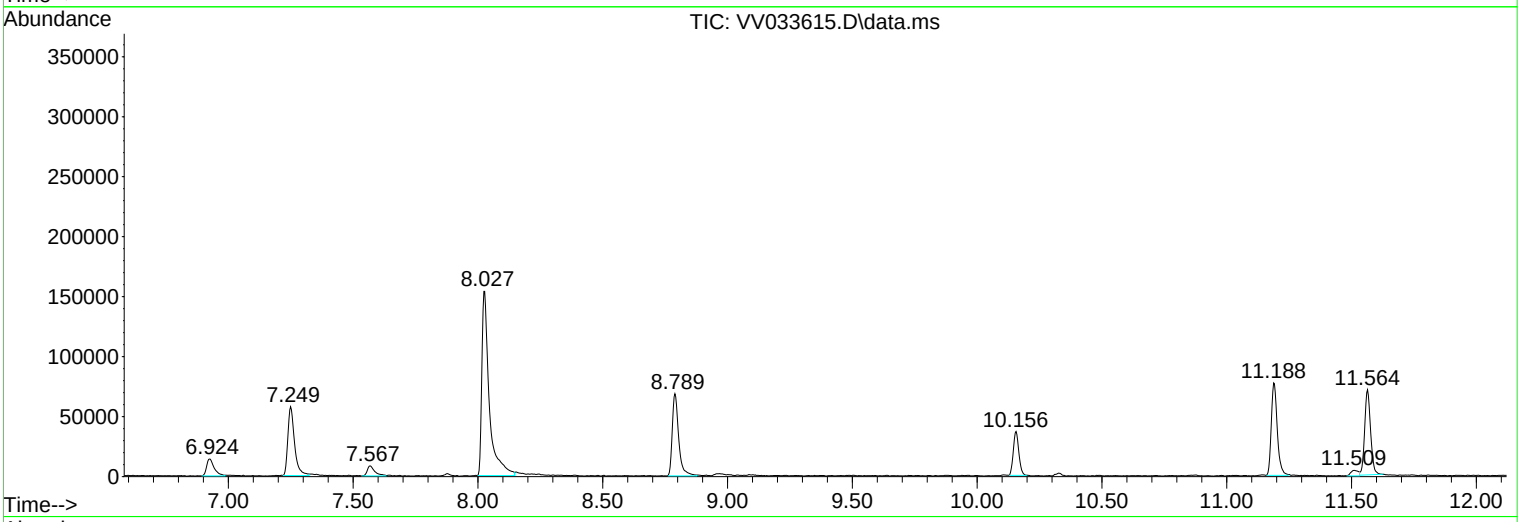
ALS Vial : 36 Sample Multiplier: 1

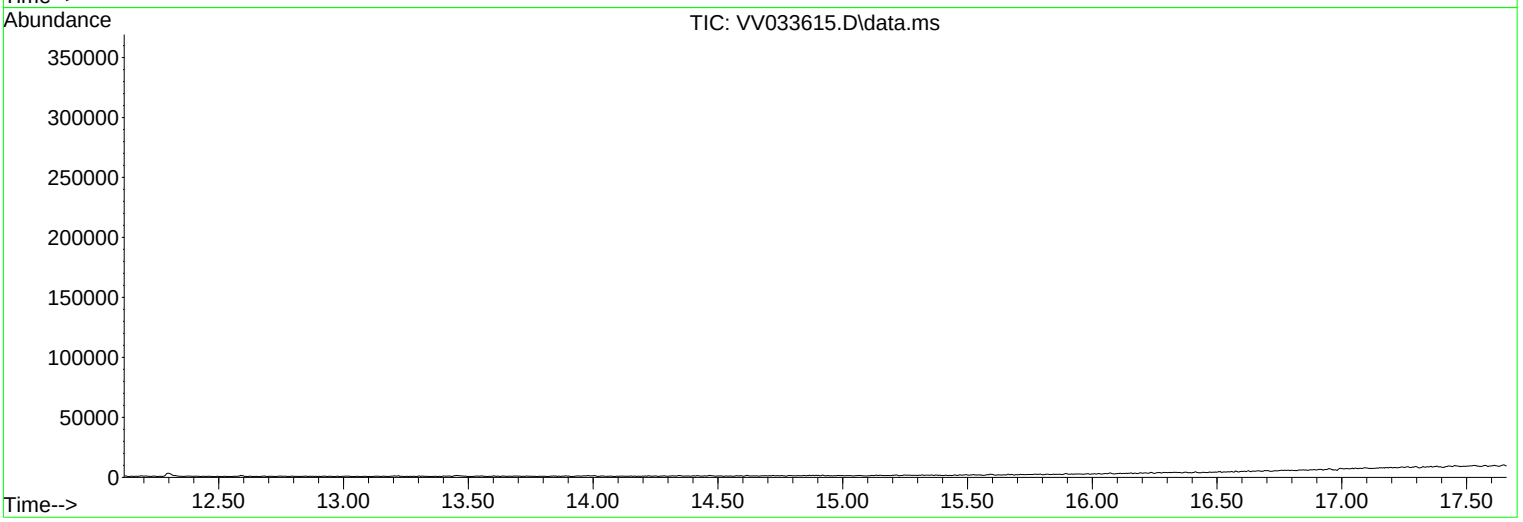
Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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







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Data File : VV033615.D
Acq On : 12 Jan 2024 23:28
Operator : SY/MD
Sample : P1121-07
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ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

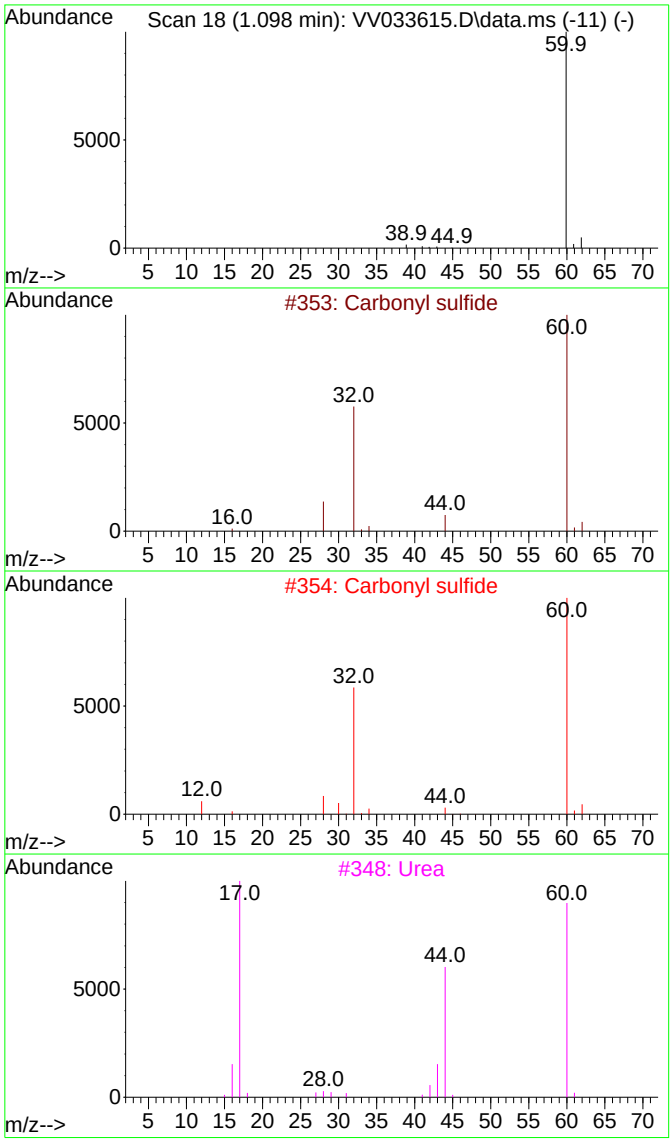
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

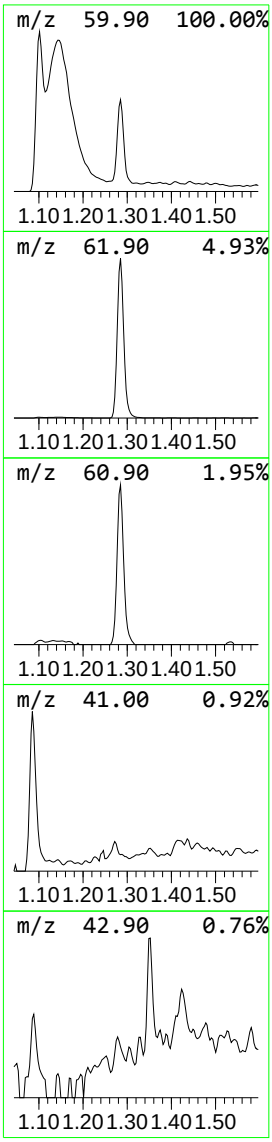
****

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.098	0.75 ug/L	13878	1,4-Difluorobenzene	5.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonyl sulfide	60	COS	000463-58-1	5
2	Carbonyl sulfide	60	COS	000463-58-1	5
3	Urea	60	CH4N2O	000057-13-6	4
4	Thiirane	60	C2H4S	000420-12-2	4
5	Urea	60	CH4N2O	000057-13-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011224\
Data File : VV033615.D
Acq On : 12 Jan 2024 23:28
Operator : SY/MD
Sample : P1121-07
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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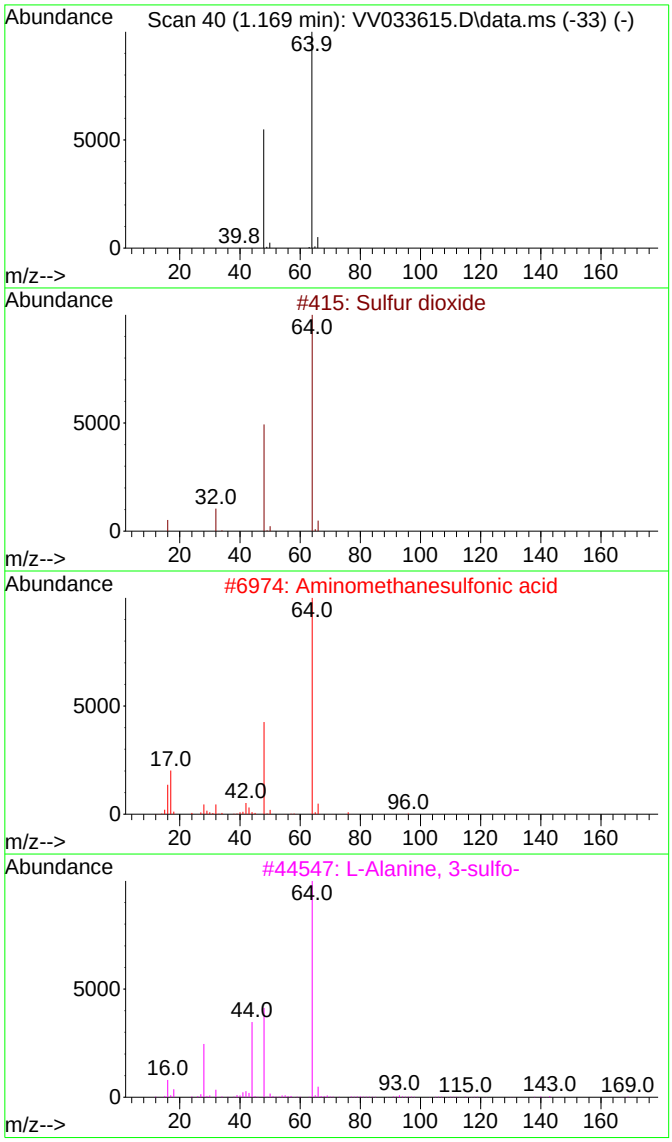
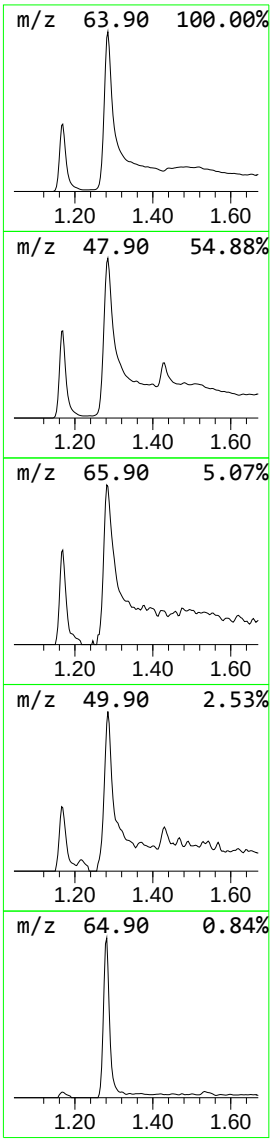
Peak Number 2 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.169	6.40 ug/L	118323	1,4-Difluorobenzene	5.542

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011224\
Data File : VV033615.D
Acq On : 12 Jan 2024 23:28
Operator : SY/MD
Sample : P1121-07
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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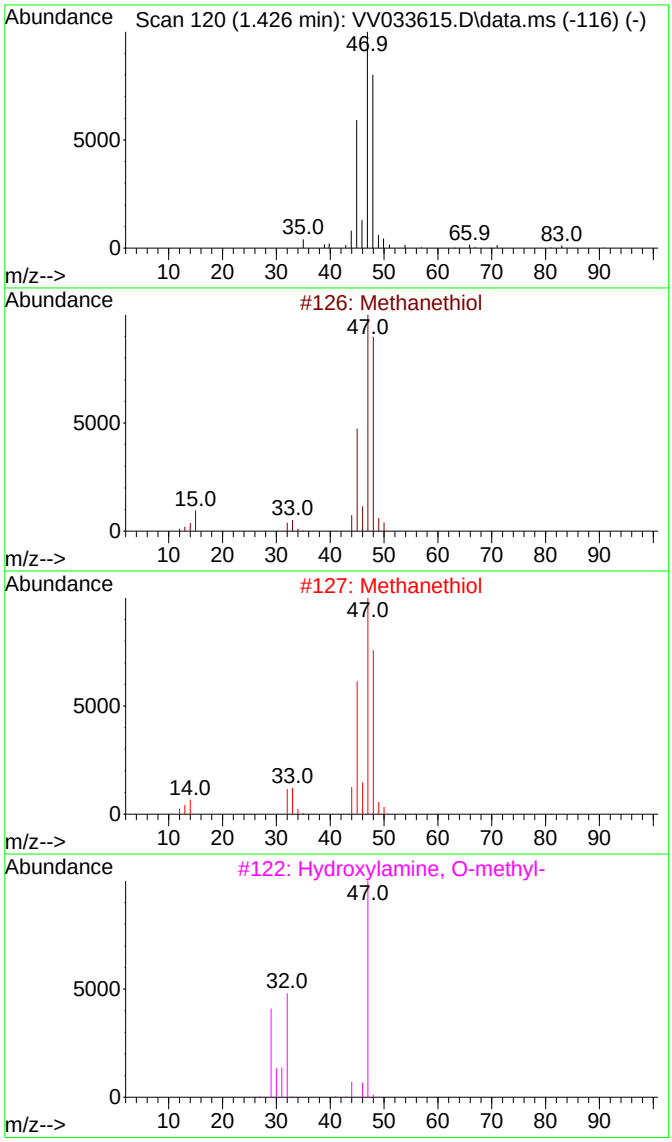
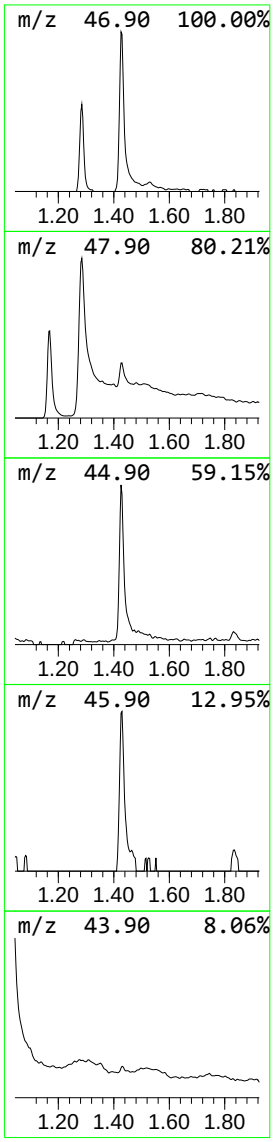
Peak Number 3 Methanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.426	1.48 ug/L	27390	1,4-Difluorobenzene	5.542

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011224\
Data File : VV033615.D
Acq On : 12 Jan 2024 23:28
Operator : SY/MD
Sample : P1121-07
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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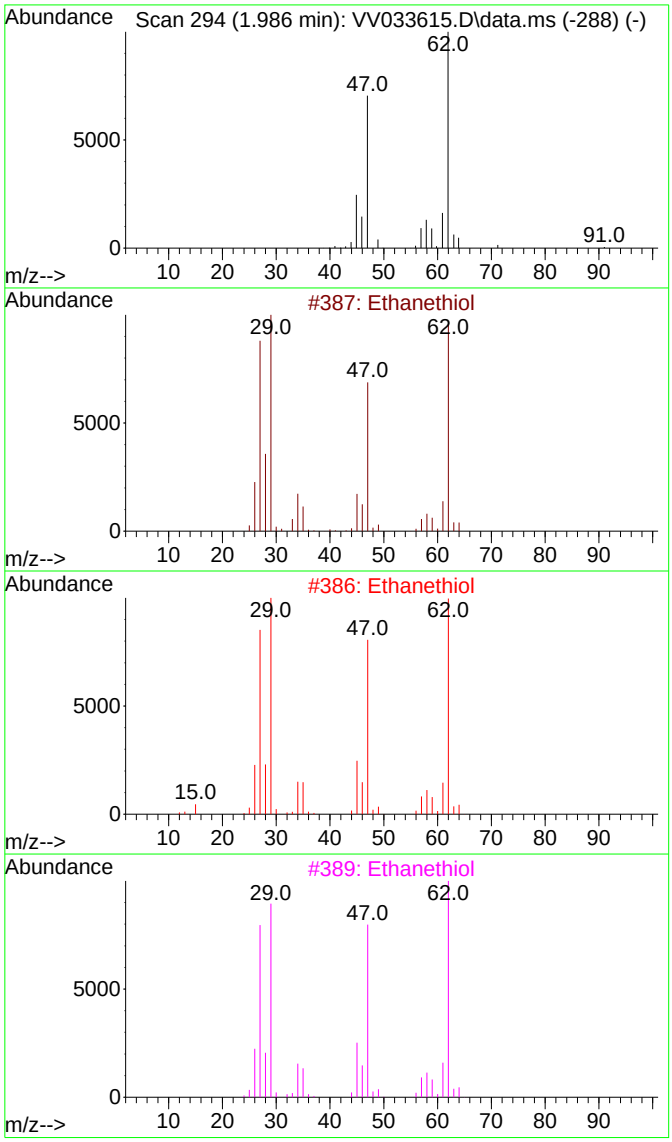
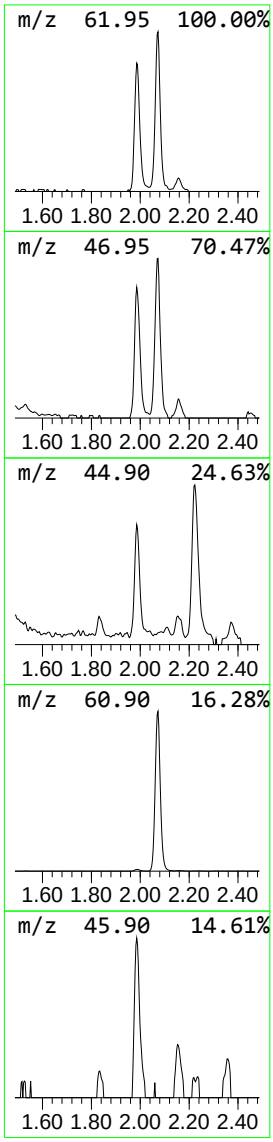
Peak Number 4 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.986	2.11 ug/L	38949	1,4-Difluorobenzene	5.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol	62	C2H6S	000075-08-1	91
2	Ethanethiol	62	C2H6S	000075-08-1	90
3	Ethanethiol	62	C2H6S	000075-08-1	90
4	Ethanethiol	62	C2H6S	000075-08-1	87
5	Ethanethiol	62	C2H6S	000075-08-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011224\
Data File : VV033615.D
Acq On : 12 Jan 2024 23:28
Operator : SY/MD
Sample : P1121-07
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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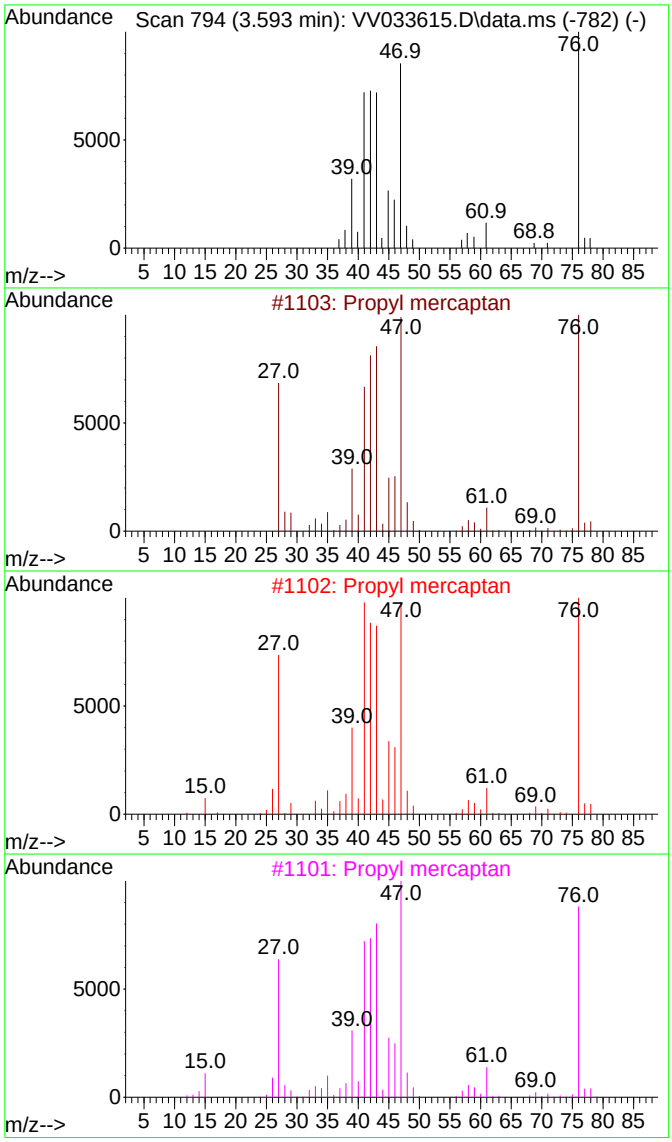
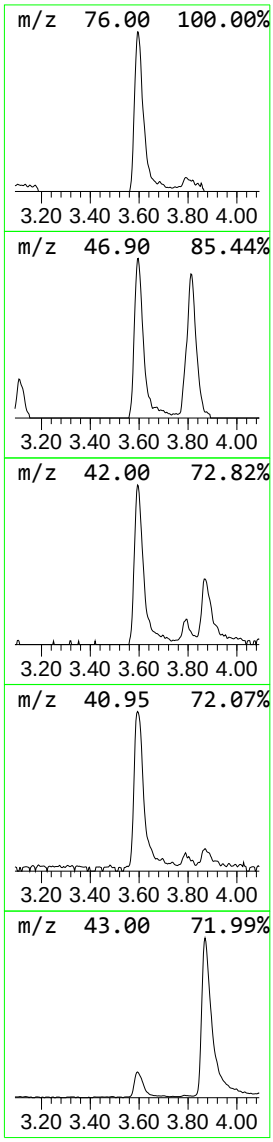
Peak Number 5 Propyl mercaptan Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.593	4.96 ug/L	91759	1,4-Difluorobenzene	5.542

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	96
3	Propyl mercaptan	76	C3H8S	000107-03-9	96
4	Propyl mercaptan	76	C3H8S	000107-03-9	95
5	Propyl mercaptan	76	C3H8S	000107-03-9	91





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Operator : SY/MD
Sample : P1121-07
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ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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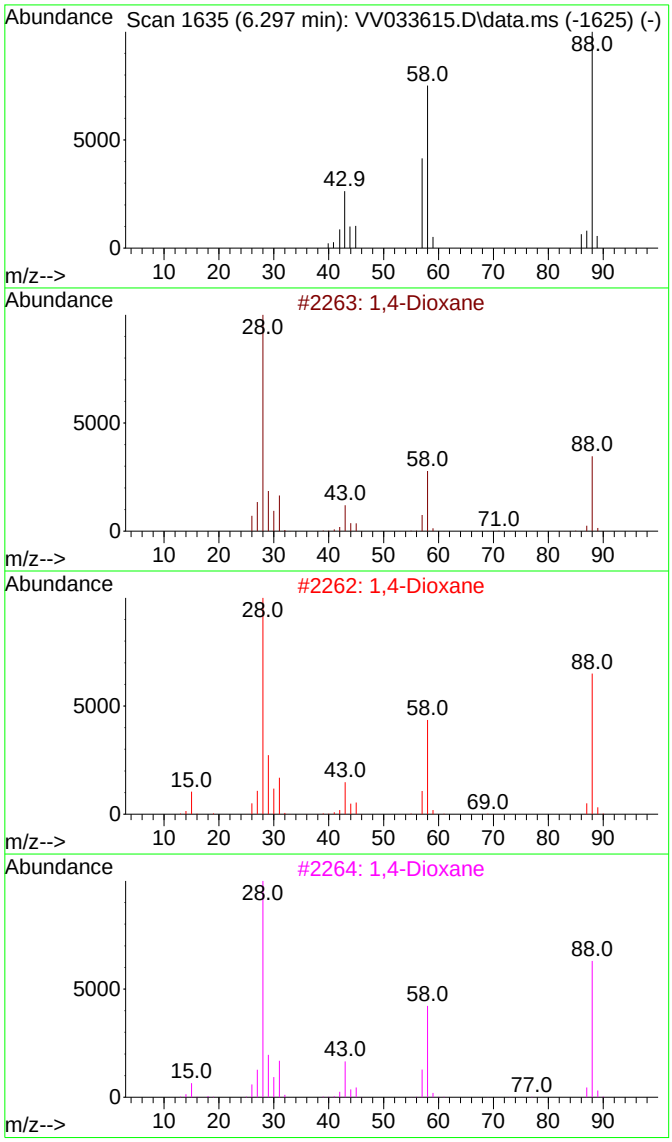
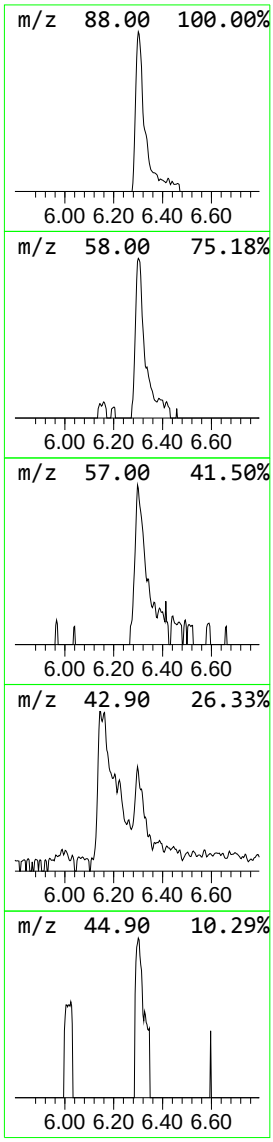
Peak Number 6 1,4-Dioxane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.297	0.90 ug/L	16555	1,4-Difluorobenzene	5.542

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Dioxane	88	C4H8O2	000123-91-1	91
2	1,4-Dioxane	88	C4H8O2	000123-91-1	90
3	1,4-Dioxane	88	C4H8O2	000123-91-1	90
4	1,4-Dioxane	88	C4H8O2	000123-91-1	90
5	Urea, N,N'-dimethyl-	88	C3H8N2O	000096-31-1	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011224\
Data File : VV033615.D
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ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8L0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
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
unknown-01	1.098	0.8	ug/L	13878	1	5.542	92452	5.0
Sulfur dioxide	1.169	6.4	ug/L	118323	1	5.542	92452	5.0
Methanethiol	1.426	1.5	ug/L	27390	1	5.542	92452	5.0
Ethanethiol	1.986	2.1	ug/L	38949	1	5.542	92452	5.0
Propyl mercaptan	3.593	5.0	ug/L	91759	1	5.542	92452	5.0
1,4-Dioxane	6.297	0.9	ug/L	16555	1	5.542	92452	5.0