

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110222\
 Data File : VU051719.D
 Acq On : 03 Nov 2022 03:33
 Operator : JC/MD
 Sample : N5301-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWN4

Integration Parameters: rteint.p

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.1
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051719.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.391	11	16	26	rVB3	10586	15125	2.24%	0.217%
2	1.507	40	52	53	rBV2	54585	88860	13.19%	1.277%
3	1.594	74	79	86	rBV	91603	111895	16.61%	1.608%
4	1.787	132	139	156	rVB	459801	606488	90.02%	8.713%
5	2.562	369	380	399	rVB	138076	221427	32.86%	3.181%
6	2.681	407	417	436	rVB2	36505	69556	10.32%	0.999%
7	2.787	441	450	463	rVB	14835	26407	3.92%	0.379%
8	3.350	617	625	641	rVB4	14999	30862	4.58%	0.443%
9	3.697	730	733	757	rVB	8367	20575	3.05%	0.296%
10	3.841	761	778	791	rVB	5077	14424	2.14%	0.207%
11	4.661	1015	1033	1054	rBV4	104893	345100	51.22%	4.958%
12	5.060	1137	1157	1179	rBV2	132762	305644	45.36%	4.391%
13	5.722	1343	1363	1392	rBV2	254398	663082	98.42%	9.526%
14	6.247	1510	1526	1550	rBV	199874	387962	57.58%	5.574%
15	6.542	1606	1618	1632	rBV2	39577	77068	11.44%	1.107%
16	6.690	1650	1664	1680	rBV	163430	324434	48.15%	4.661%
17	6.761	1680	1686	1698	rVB4	5648	10100	1.50%	0.145%
18	7.195	1809	1821	1829	rBV6	4255	8332	1.24%	0.120%
19	7.565	1923	1936	1954	rBV	67998	122995	18.26%	1.767%
20	7.677	1960	1971	1997	rBV3	27882	61918	9.19%	0.890%
21	7.896	2027	2039	2055	rBV	273829	476424	70.71%	6.845%
22	7.967	2058	2061	2073	rVB4	6982	10527	1.56%	0.151%
23	8.179	2114	2127	2141	rBV2	42533	75931	11.27%	1.091%
24	8.472	2209	2218	2238	rBV5	10683	29842	4.43%	0.429%
25	8.636	2257	2269	2298	rBV	313772	673752	100.00%	9.680%
26	9.417	2497	2512	2530	rBV	314488	533911	79.24%	7.671%
27	9.597	2555	2568	2580	rBV	11993	19449	2.89%	0.279%
28	10.012	2685	2697	2719	rBV4	31186	97894	14.53%	1.406%
29	10.092	2720	2722	2737	rVB8	4361	8032	1.19%	0.115%
30	10.462	2824	2837	2855	rVB5	6152	12226	1.81%	0.176%
31	10.754	2916	2928	2948	rBV	142012	235047	34.89%	3.377%
32	10.889	2960	2970	2980	rVB	9677	14869	2.21%	0.214%
33	11.362	3103	3117	3142	rBV2	27891	58548	8.69%	0.841%
34	11.812	3244	3257	3275	rBV	309466	505314	75.00%	7.260%
35	12.063	3322	3335	3359	rVB4	23411	50751	7.53%	0.729%
36	12.192	3359	3375	3394	rBV	283454	470775	69.87%	6.764%

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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

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37	12.552	3477	3487	3499	rBV9	5822	11203	1.66%	0.161%
38	13.108	3654	3660	3667	rBV6	4745	6911	1.03%	0.099%
39	13.619	3808	3819	3831	rBV6	25593	44334	6.58%	0.637%
40	14.098	3957	3968	3975	rBV4	11143	17564	2.61%	0.252%
41	14.143	3975	3982	3990	rVB2	12014	17004	2.52%	0.244%
42	14.613	4118	4128	4142	rVB4	25488	43364	6.44%	0.623%
43	15.545	4407	4418	4429	rBV6	20835	34561	5.13%	0.497%

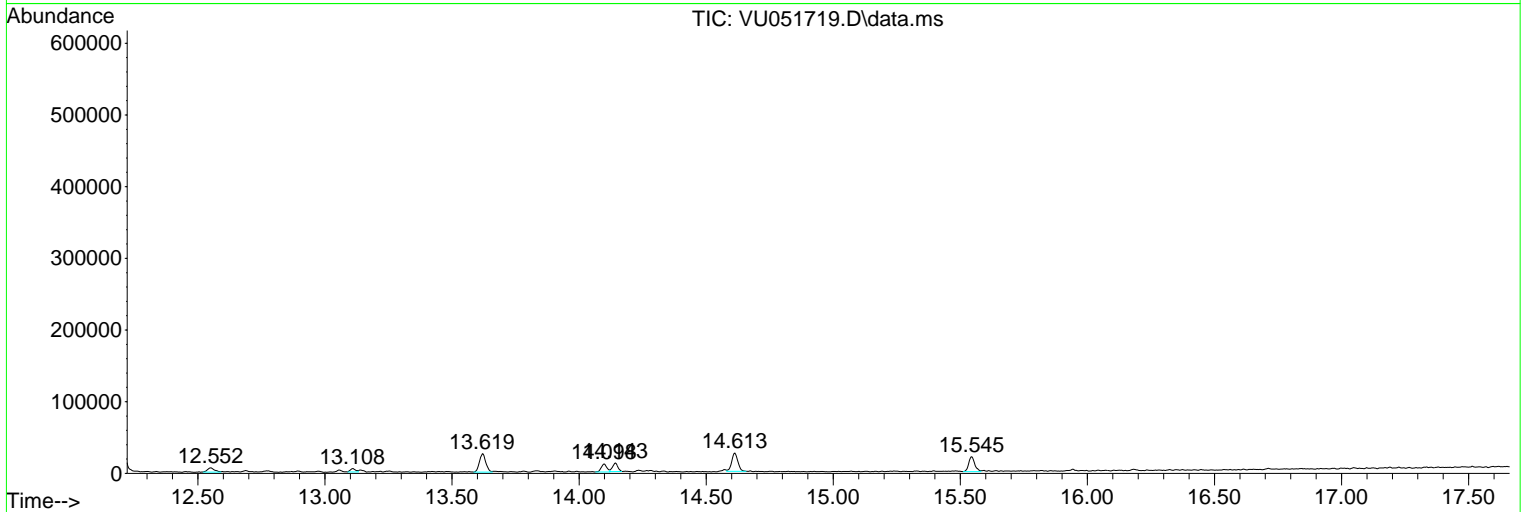
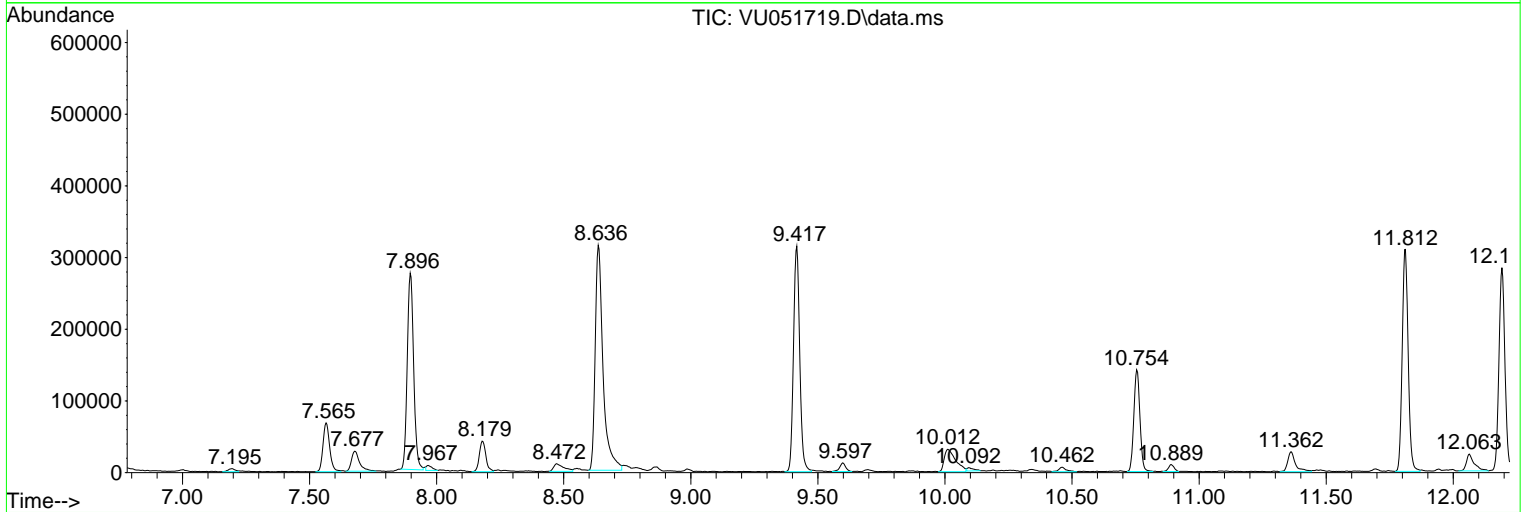
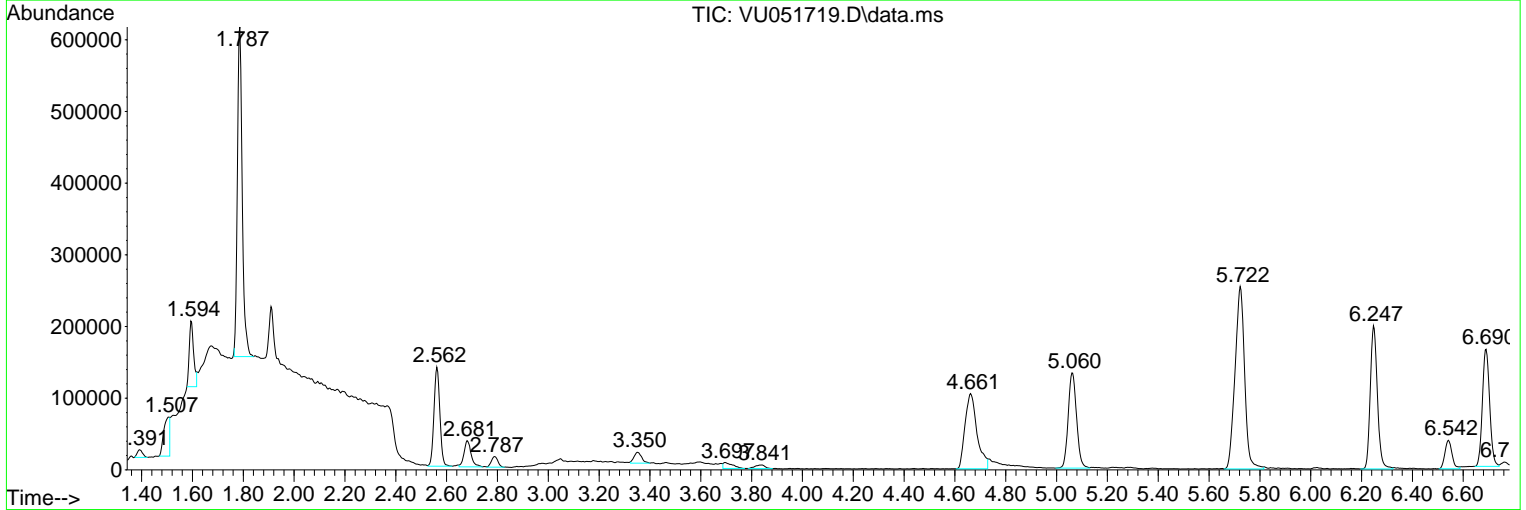
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Quant Title : TRACE VOA SFAM1.0

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



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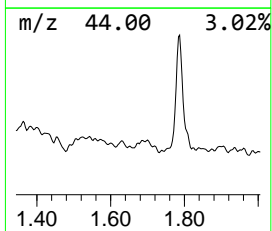
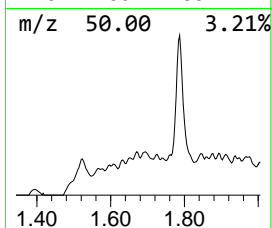
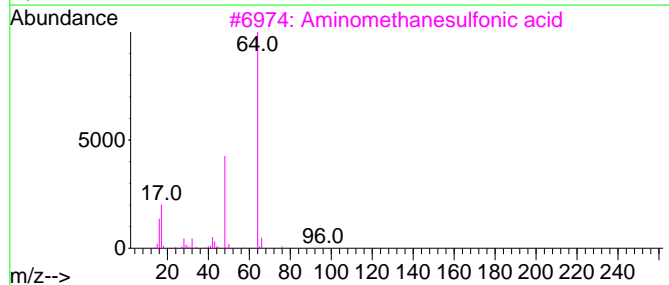
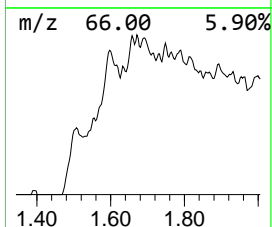
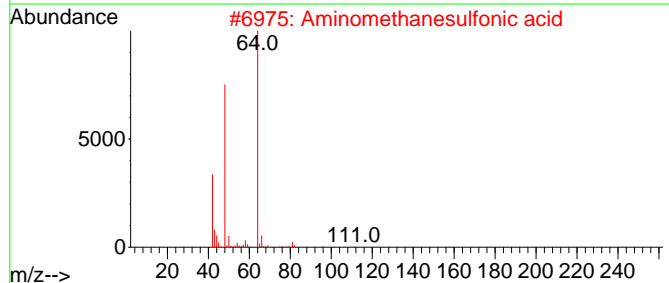
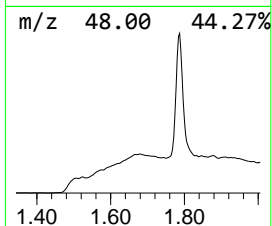
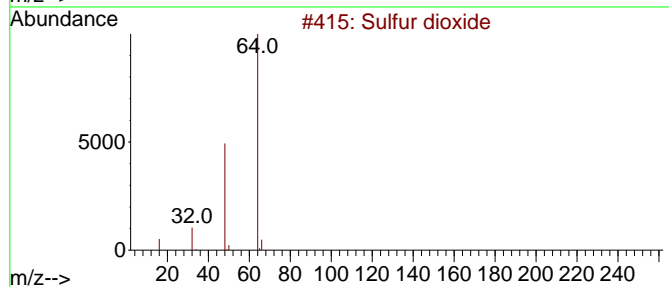
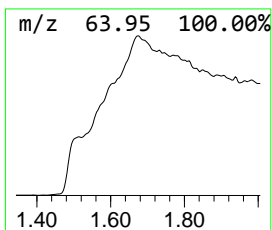
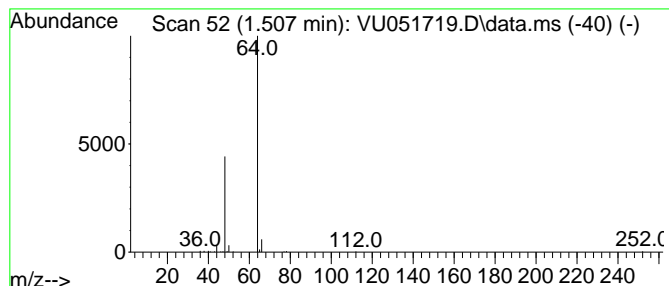
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.507	1.15 ug/L	88860	1,4-Difluorobenzene	6.247

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	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
5			1,1,1,2,2,3,3,4,4,5,5-Undecafluoro...	602	C10F22O2S	1000486-78-5	64



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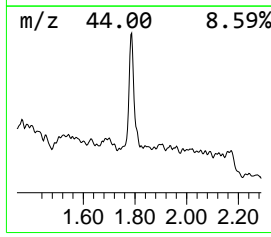
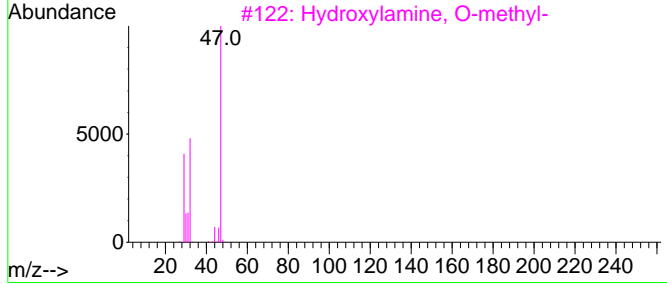
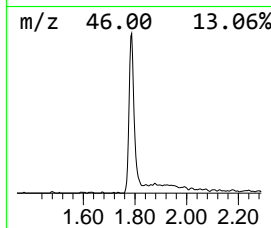
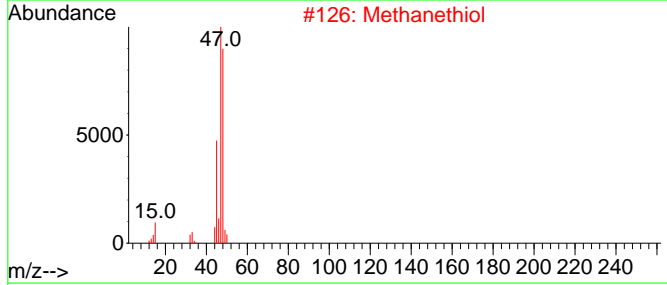
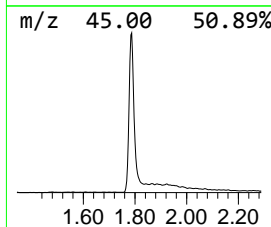
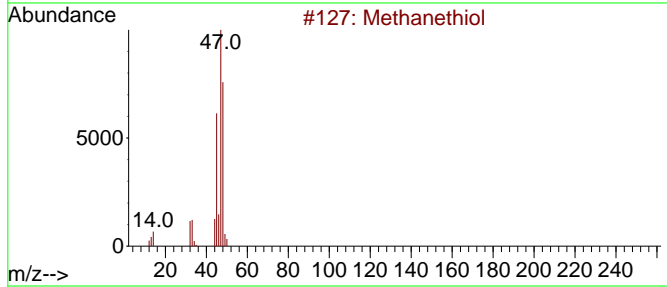
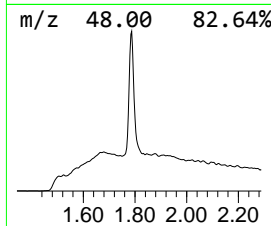
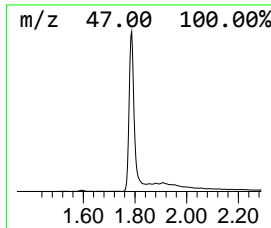
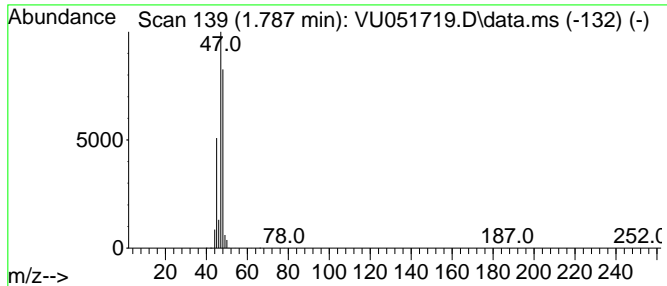
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 2 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.787	7.82 ug/L	606488	1,4-Difluorobenzene	6.247

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Ethanol	46	C2H6O	000064-17-5	4



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Instrument :
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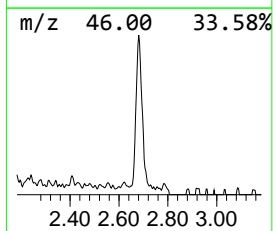
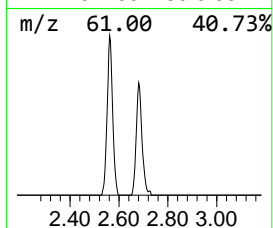
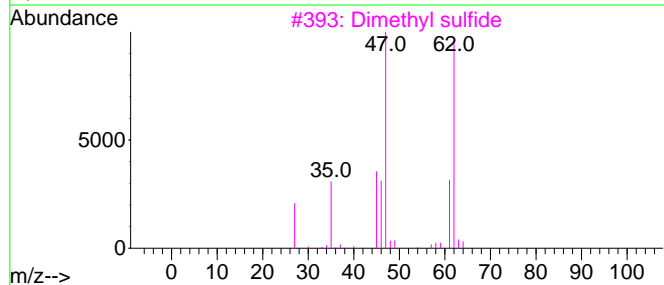
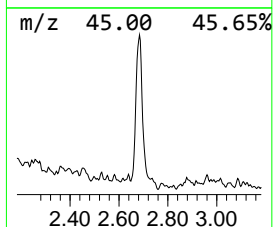
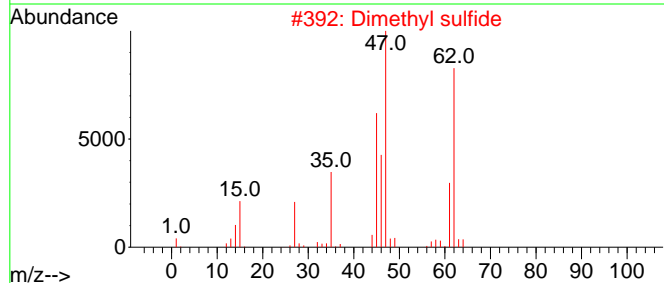
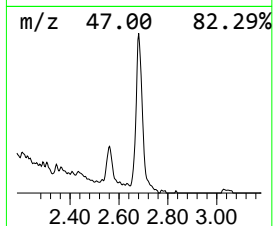
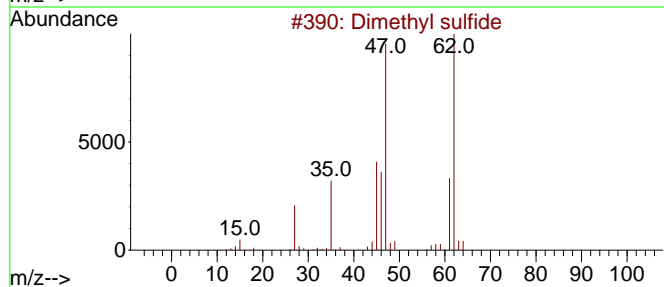
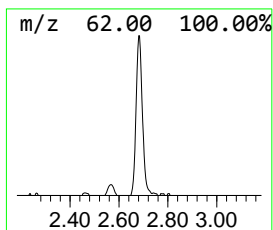
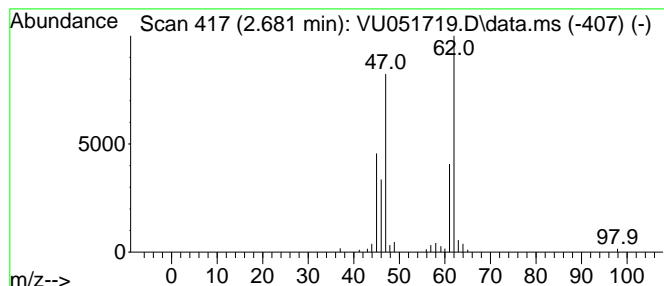
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 3 Dimethyl sulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.681	0.90 ug/L	69556	1,4-Difluorobenzene	6.247

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	Dimethyl sulfide	62	C2H6S	000075-18-3	91
5	Dimethyl sulfide	62	C2H6S	000075-18-3	91



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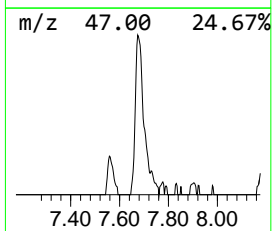
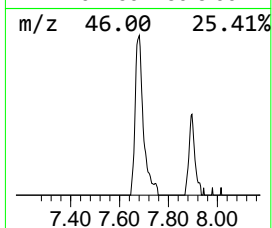
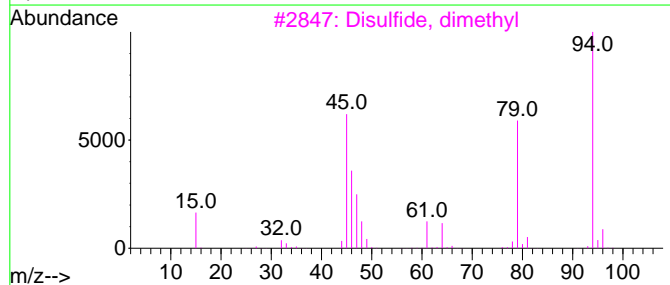
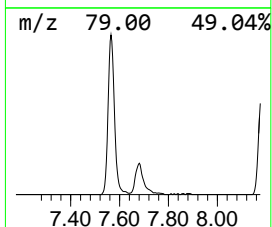
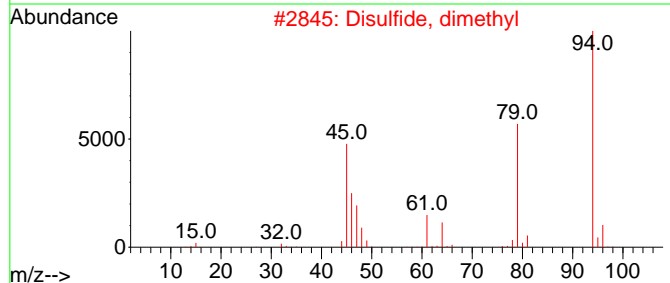
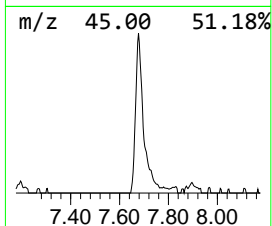
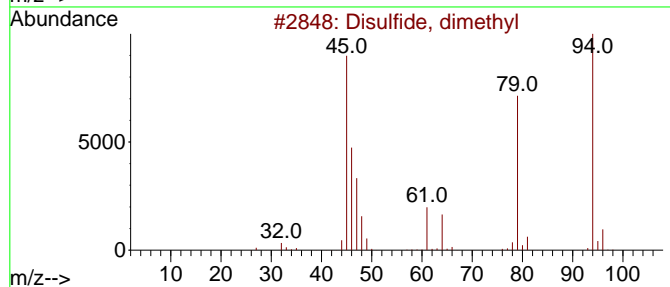
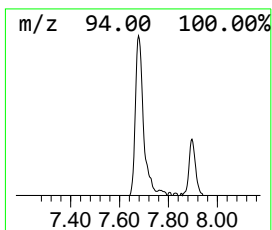
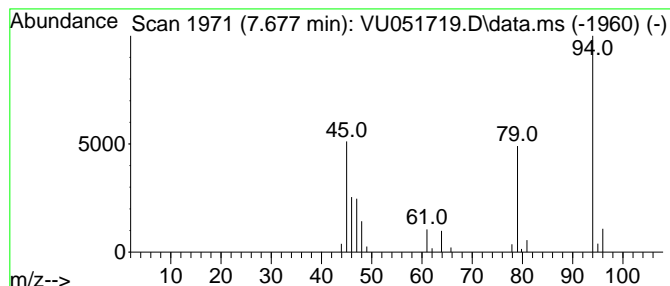
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 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 5 Disulfide, dimethyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.677	0.80 ug/L	61918	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	95
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	83



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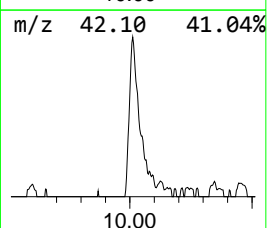
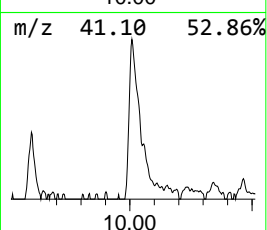
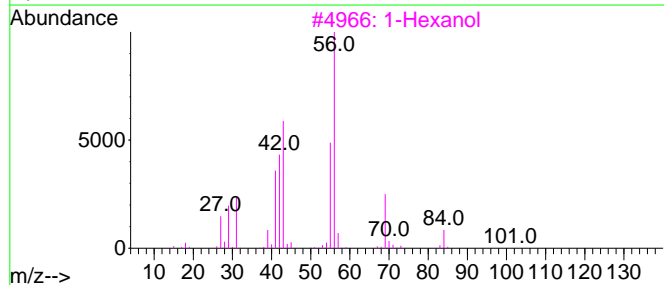
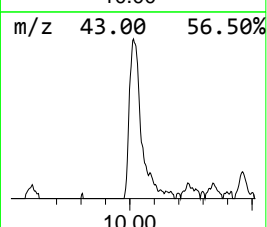
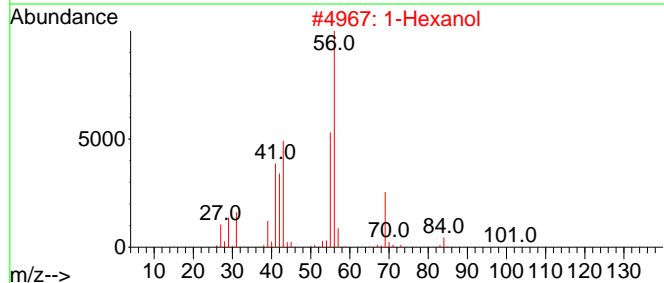
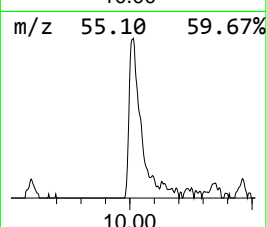
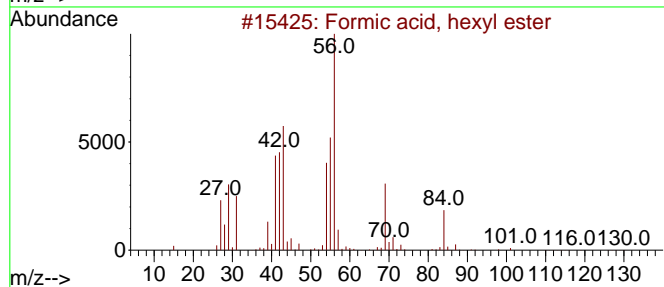
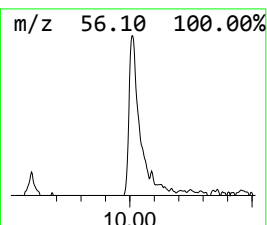
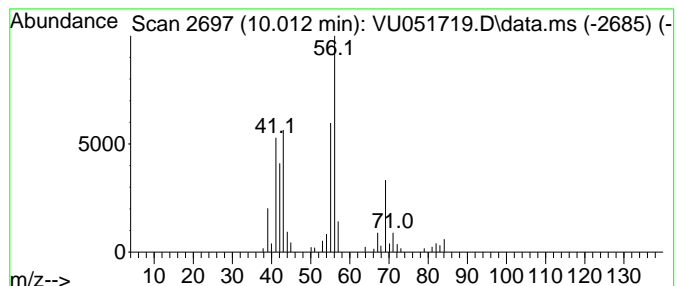
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 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 6 Formic acid, hexyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.012	0.92 ug/L	97894	Chlorobenzene-d5	9.417

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
2		1-Hexanol	102	C6H14O	000111-27-3	72
3		1-Hexanol	102	C6H14O	000111-27-3	72
4		1-Hexanol	102	C6H14O	000111-27-3	72
5		1-Hexanol	102	C6H14O	000111-27-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110222\
 Data File : VU051719.D
 Acq On : 03 Nov 2022 03:33
 Operator : JC/MD
 Sample : N5301-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWN4

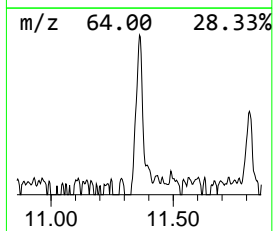
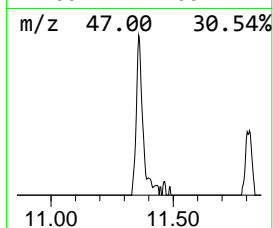
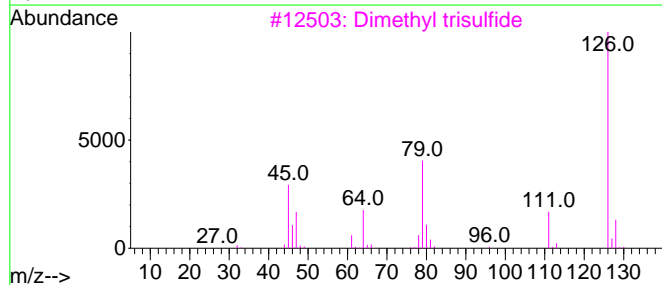
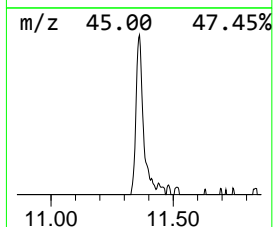
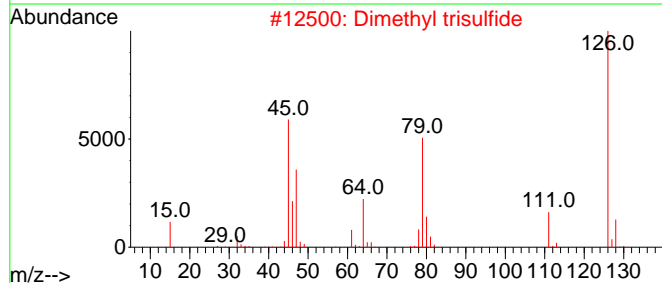
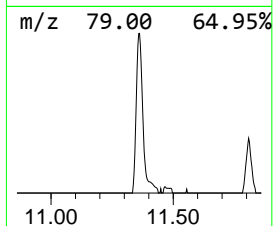
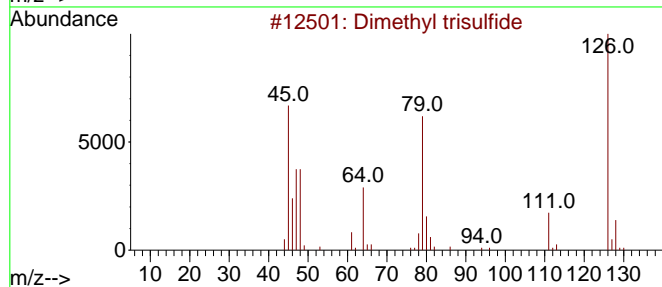
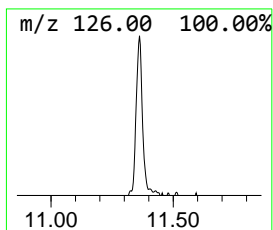
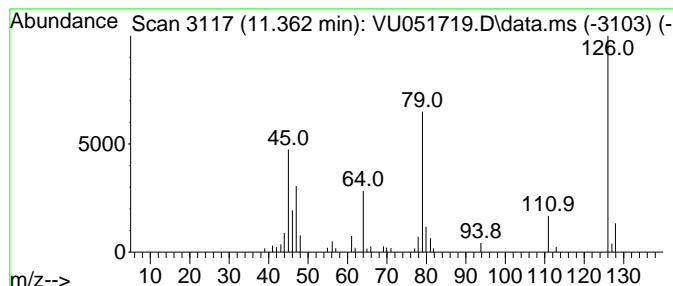
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 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 7 Dimethyl trisulfide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.362	0.58 ug/L	58548	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl trisulfide	126	C2H6S3	003658-80-8	94
2			Dimethyl trisulfide	126	C2H6S3	003658-80-8	91
3			Dimethyl trisulfide	126	C2H6S3	003658-80-8	91
4			Dimethyl trisulfide	126	C2H6S3	003658-80-8	72
5			Dimethyl trisulfide	126	C2H6S3	003658-80-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110222\
 Data File : VU051719.D
 Acq On : 03 Nov 2022 03:33
 Operator : JC/MD
 Sample : N5301-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWN4

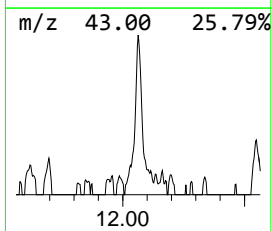
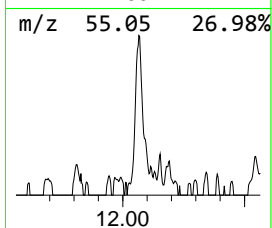
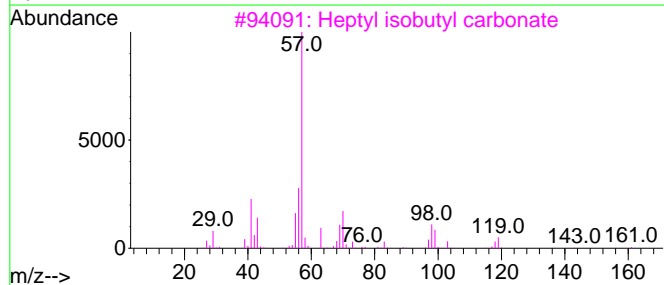
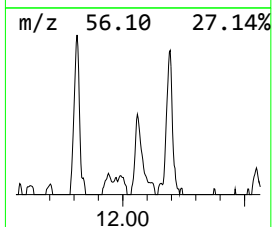
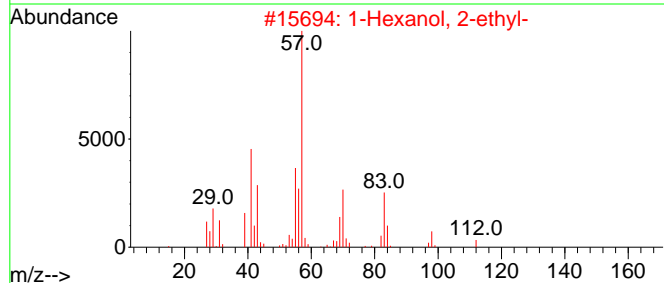
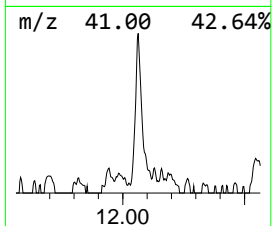
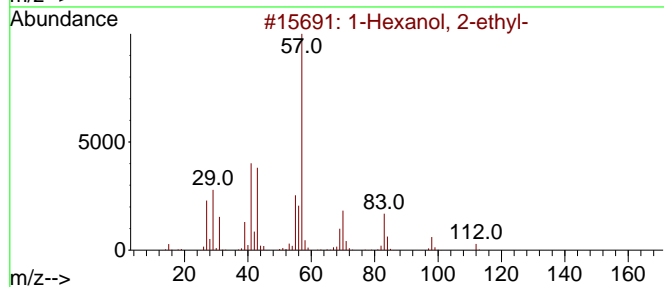
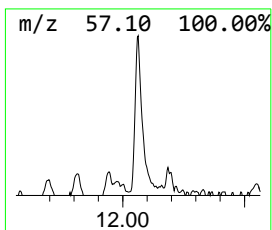
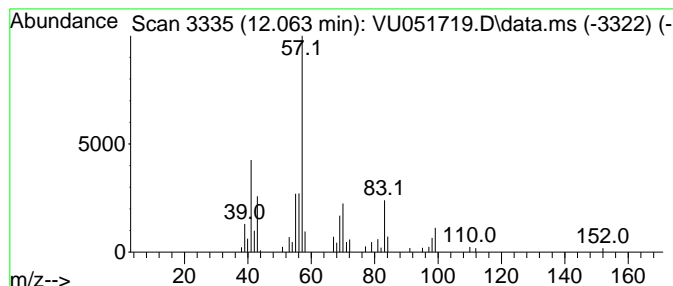
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 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	0.50 ug/L	50751	1,4-Dichlorobenzene-d4	11.812

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3		Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	53
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53
5		Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110222\
 Data File : VU051719.D
 Acq On : 03 Nov 2022 03:33
 Operator : JC/MD
 Sample : N5301-19
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWN4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
 Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.507	1.1	ug/L	88860	1	6.247	387962	5.0
Methanethiol	1.787	7.8	ug/L	606488	1	6.247	387962	5.0
Dimethyl sulfide	2.681	0.9	ug/L	69556	1	6.247	387962	5.0
Disulfide, dime...	7.677	0.8	ug/L	61918	1	6.247	387962	5.0
Formic acid, he...	10.012	0.9	ug/L	97894	2	9.417	533911	5.0
Dimethyl trisul...	11.362	0.6	ug/L	58548	3	11.812	505314	5.0
1-Hexanol, 2-et...	12.063	0.5	ug/L	50751	3	11.812	505314	5.0