

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
 Data File : VV026365.D
 Acq On : 17 Jun 2022 04:27
 Operator : SY/MD
 Sample : N3320-17 5X
 Misc : 25mL/MSVOA_V/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGJ92

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\SFAMVTR061522WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV026365.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.323	80	88	101	rBV2	183700	207515	9.84%	2.819%
2	1.487	123	139	143	rBV2	85804	194310	9.21%	2.639%
3	1.584	164	169	189	rVB	101797	142780	6.77%	1.939%
4	2.127	328	338	356	rVB3	277666	483136	22.91%	6.563%
5	3.208	661	674	694	rBV	62464	132557	6.29%	1.801%
6	3.703	814	828	852	rBV3	25584	70871	3.36%	0.963%
7	3.925	879	897	960	rBV	780015	2108701	100.00%	28.643%
8	4.362	1018	1033	1065	rVB2	107277	268646	12.74%	3.649%
9	5.060	1232	1250	1281	rBV2	228876	566103	26.85%	7.690%
10	5.625	1413	1426	1456	rBV	216357	445399	21.12%	6.050%
11	5.921	1506	1518	1544	rVB2	114971	232522	11.03%	3.158%
12	6.076	1553	1566	1591	rVB2	132448	268928	12.75%	3.653%
13	6.992	1838	1851	1869	rBV2	37430	74287	3.52%	1.009%
14	7.320	1942	1953	1973	rBV	251052	439138	20.83%	5.965%
15	8.095	2181	2194	2224	rBV	148987	317575	15.06%	4.314%
16	8.854	2419	2430	2456	rBV	323306	523600	24.83%	7.112%
17	10.217	2841	2854	2867	rBV	82495	129416	6.14%	1.758%
18	11.249	3164	3175	3200	rBV	273817	427930	20.29%	5.813%
19	11.622	3280	3291	3315	rBV	205192	328596	15.58%	4.463%

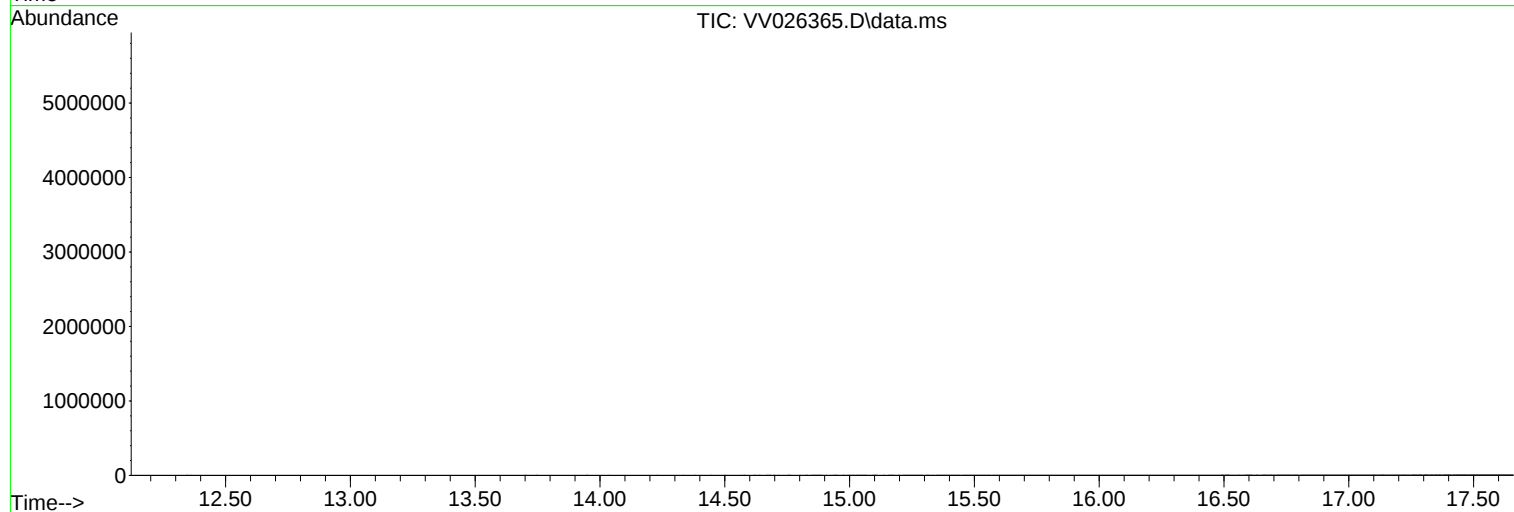
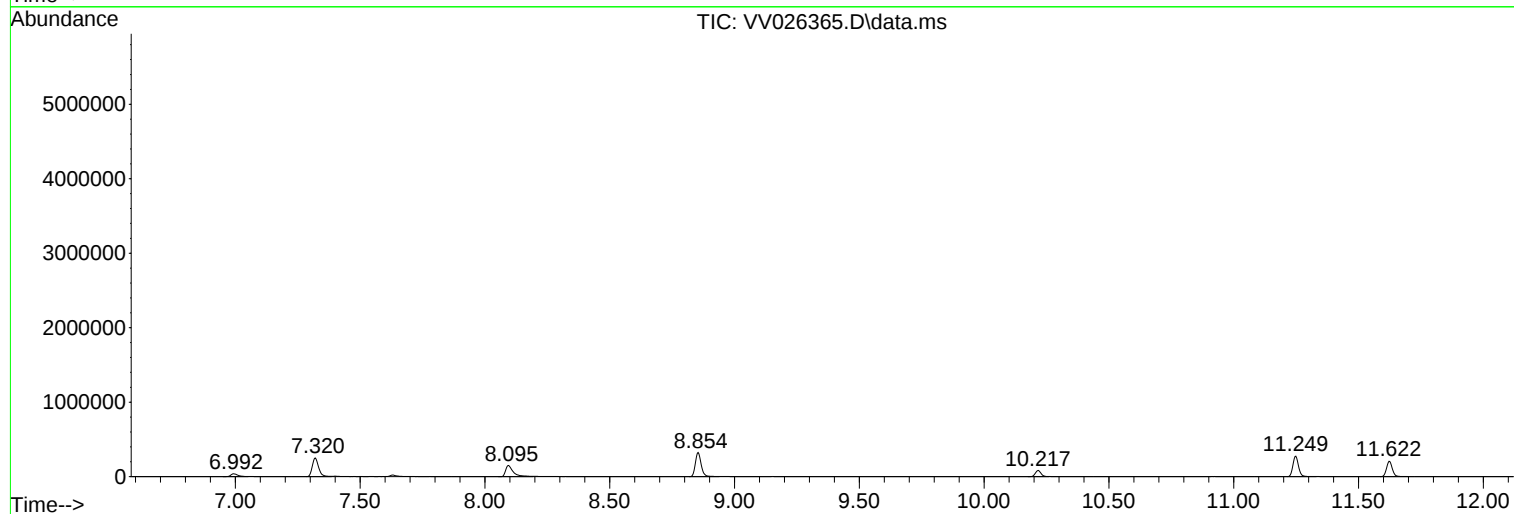
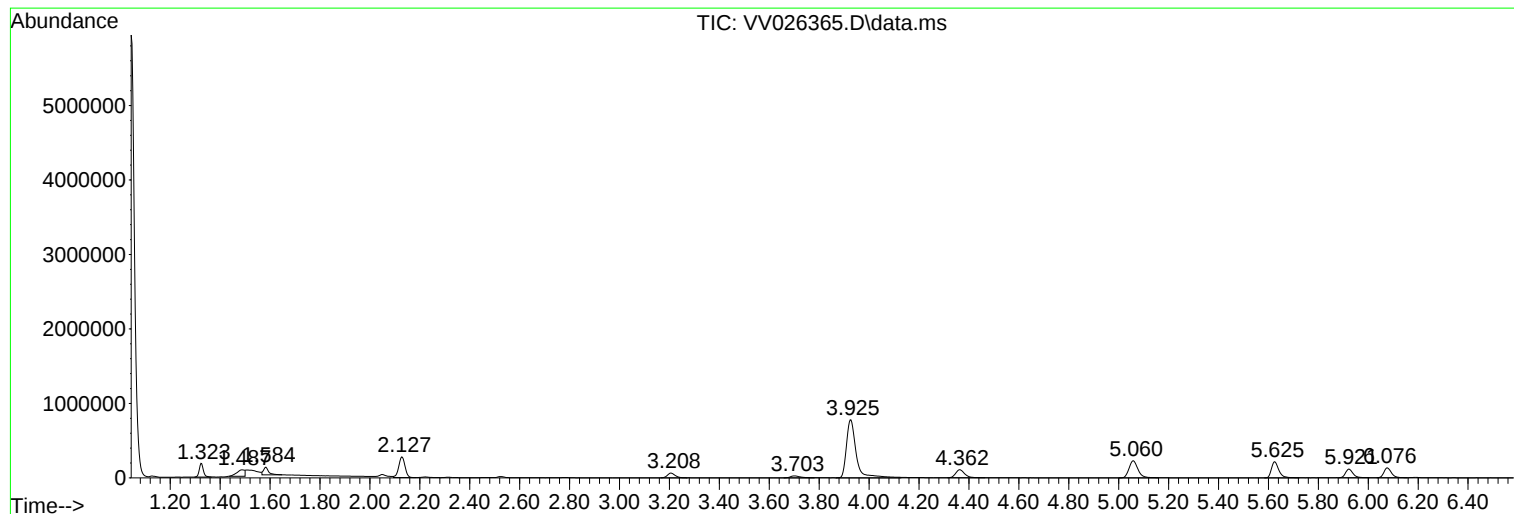
Sum of corrected areas: 7362010

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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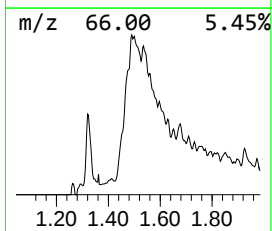
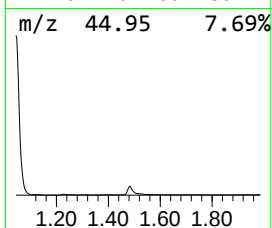
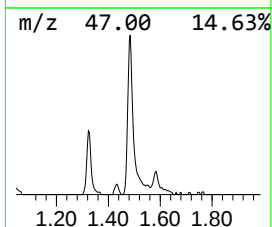
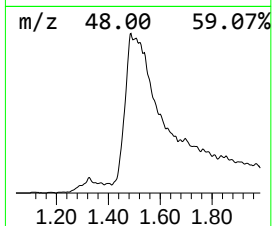
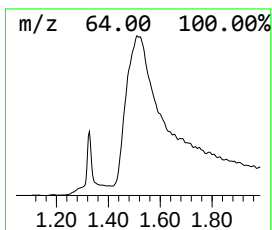
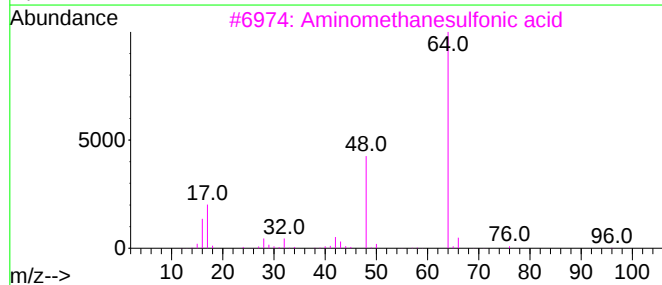
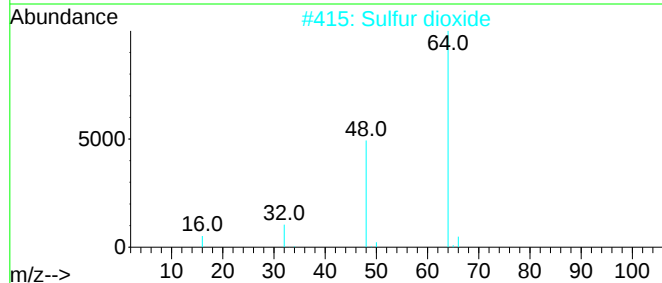
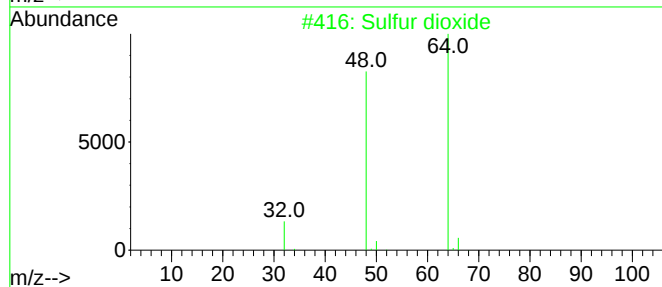
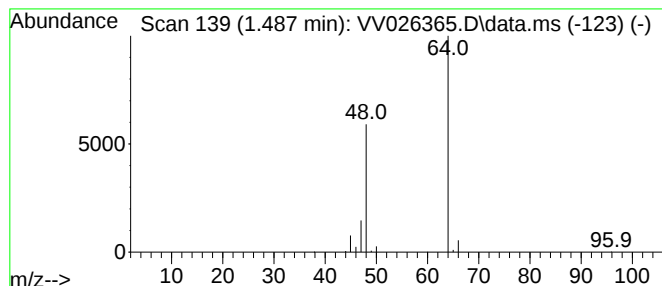
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.487	2.18 ug/L	194310	1,4-Difluorobenzene	5.625

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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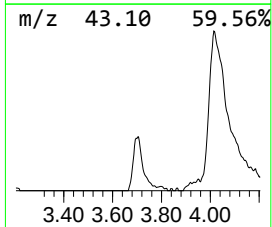
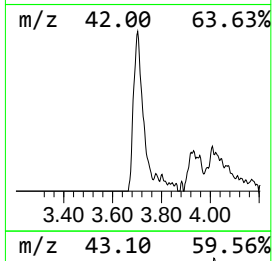
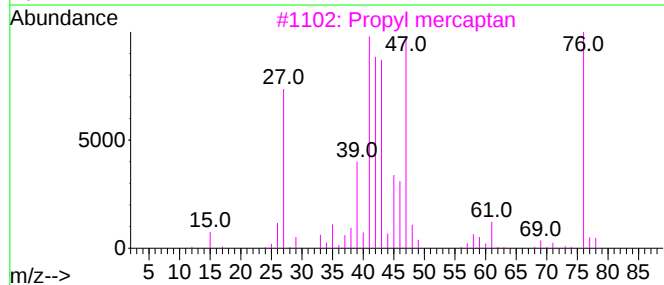
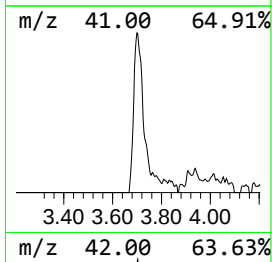
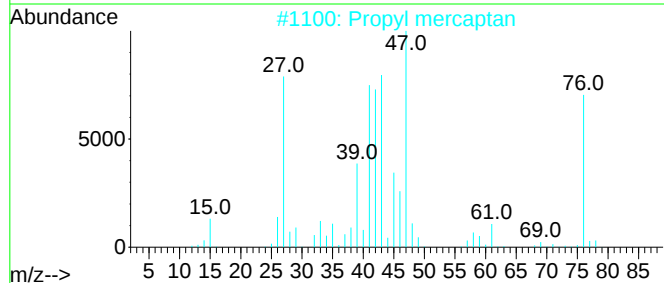
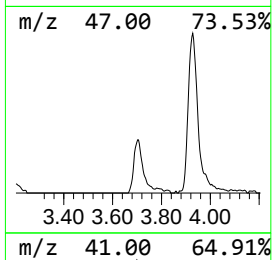
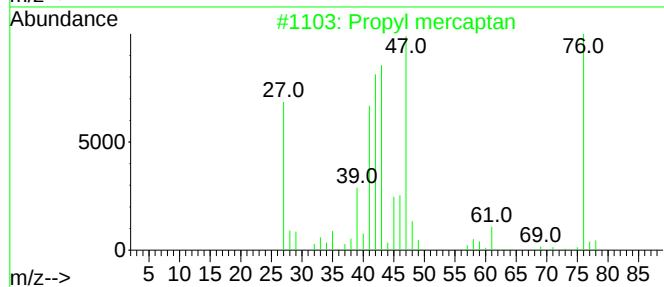
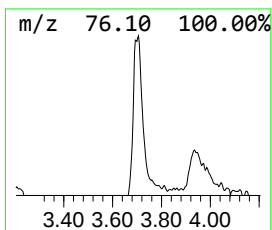
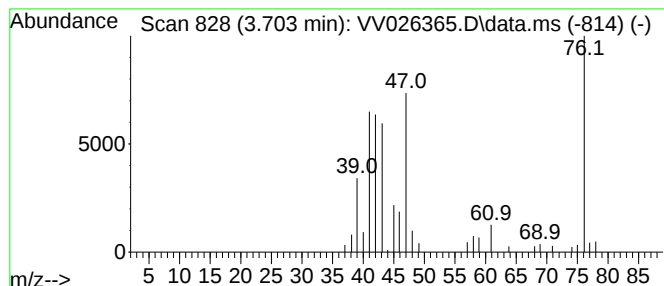
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propyl mercaptan Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.703	0.80 ug/L	70871	1,4-Difluorobenzene	5.625

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan			76	C3H8S	000107-03-9	95
2	Propyl mercaptan			76	C3H8S	000107-03-9	91
3	Propyl mercaptan			76	C3H8S	000107-03-9	91
4	Propyl mercaptan			76	C3H8S	000107-03-9	91
5	Propyl mercaptan			76	C3H8S	000107-03-9	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.487	2.2	ug/L	194310	1	5.625	445399	5.0
Propyl mercaptan	3.703	0.8	ug/L	70871	1	5.625	445399	5.0