

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV122821\
 Data File : VV024226.D
 Acq On : 28 Dec 2021 18:22
 Operator : SY/MD
 Sample : M5193-09
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0J13

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\SFAMVTR122721WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV024226.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.088	8	15	45	rBV	2363129	6158629	71.86%	28.830%
2	1.304	77	82	97	rVB2	134344	197197	2.30%	0.923%
3	1.461	124	131	148	rVB	371237	482685	5.63%	2.260%
4	2.111	322	333	349	rVB5	148679	255453	2.98%	1.196%
5	2.204	351	362	378	rBV	67490	110805	1.29%	0.519%
6	2.757	517	534	556	rBV	545161	939961	10.97%	4.400%
7	3.188	652	668	686	rBV	106365	224797	2.62%	1.052%
8	3.905	873	891	942	rBV	3580184	8570871	100.00%	40.123%
9	4.349	1015	1029	1051	rVB2	60296	148502	1.73%	0.695%
10	5.047	1229	1246	1259	rBV3	121102	297194	3.47%	1.391%
11	5.120	1259	1269	1286	rVB4	41162	99612	1.16%	0.466%
12	5.616	1412	1423	1443	rBV2	91285	184459	2.15%	0.864%
13	5.911	1498	1515	1546	rBV	1196714	2310680	26.96%	10.817%
14	6.069	1552	1564	1585	rVB2	70905	146562	1.71%	0.686%
15	7.317	1941	1952	1968	rBV	142869	252884	2.95%	1.184%
16	8.091	2184	2193	2231	rBV	104426	241689	2.82%	1.131%
17	8.850	2418	2429	2445	rBV	145202	239791	2.80%	1.123%
18	11.249	3164	3175	3192	rBV	163049	256919	3.00%	1.203%
19	11.625	3281	3292	3304	rVV	156063	242832	2.83%	1.137%

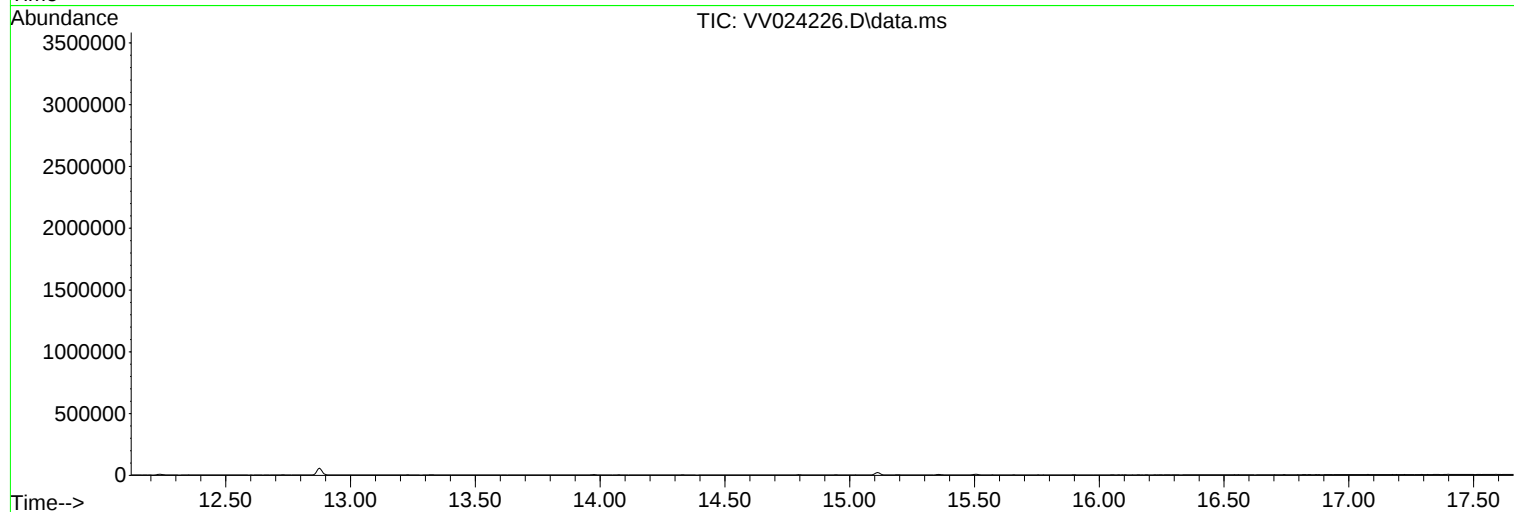
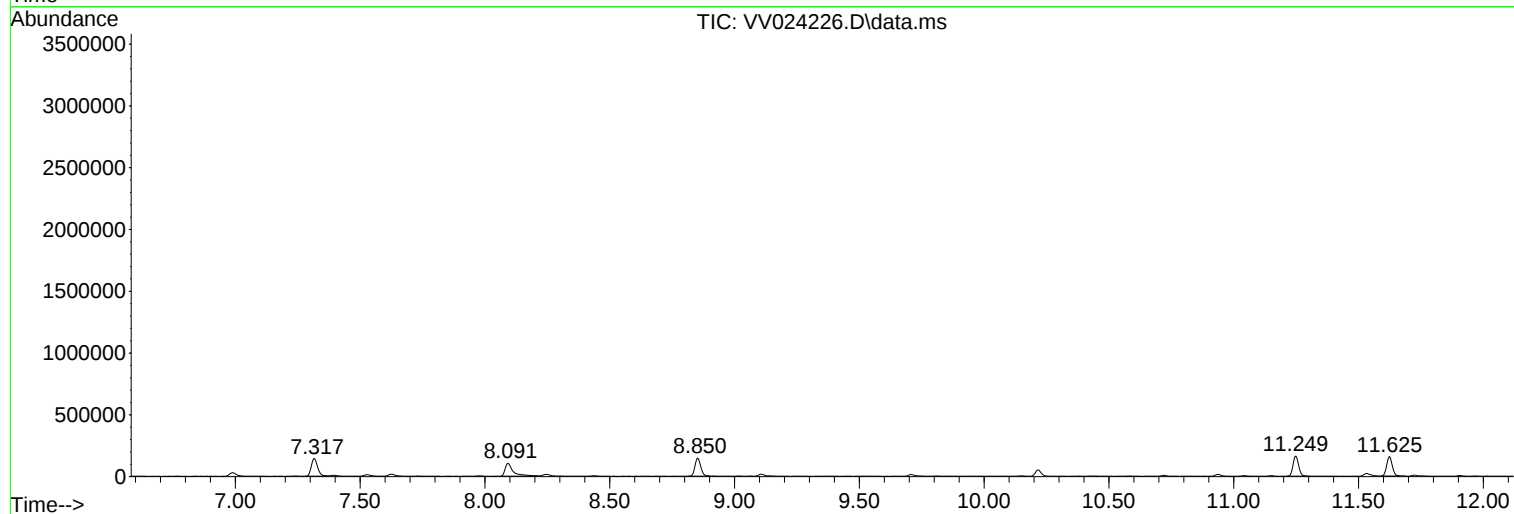
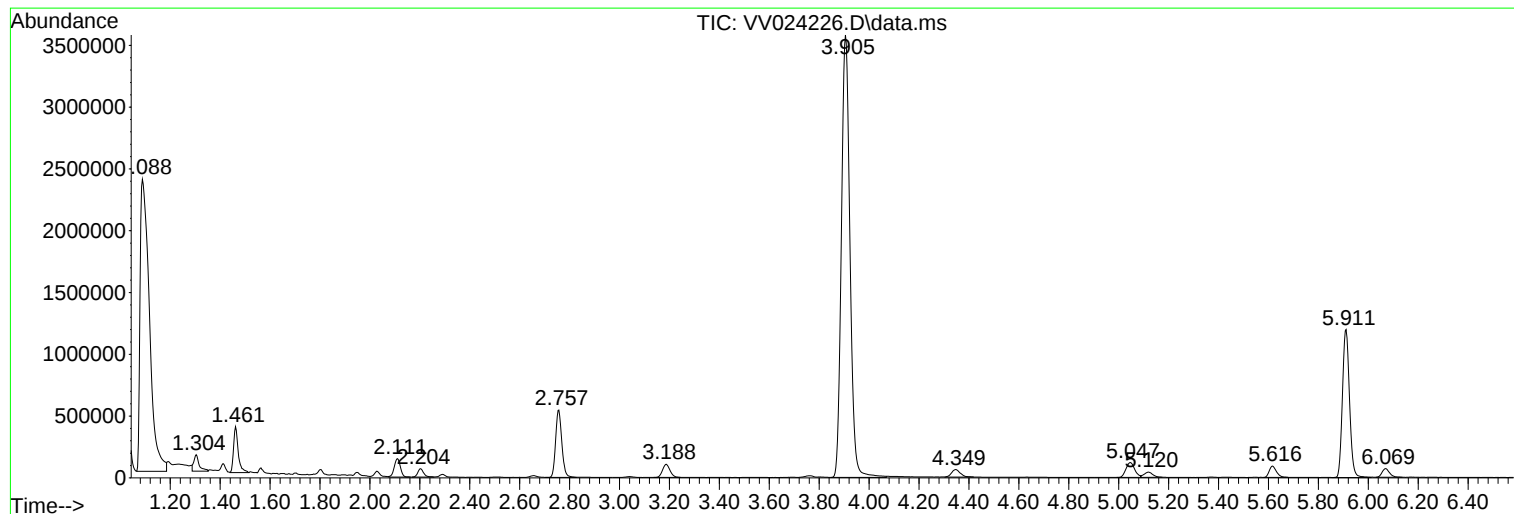
Sum of corrected areas: 21361522

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Quant Title : TRACE VOA SFAM1.0

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



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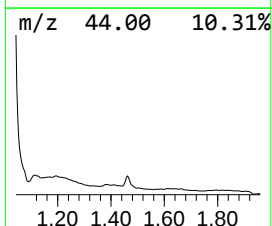
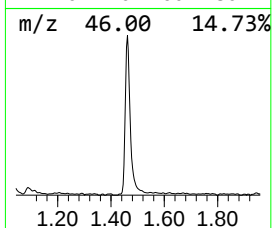
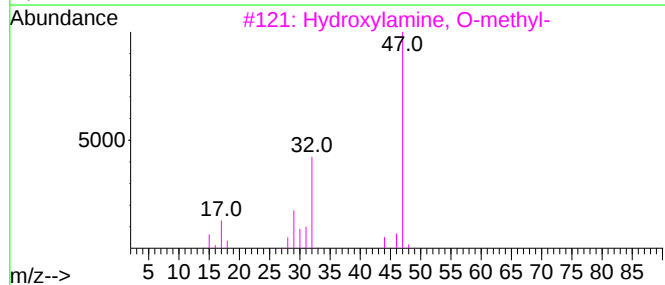
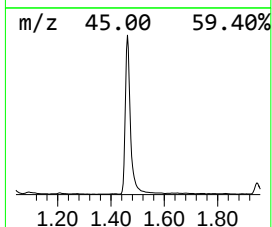
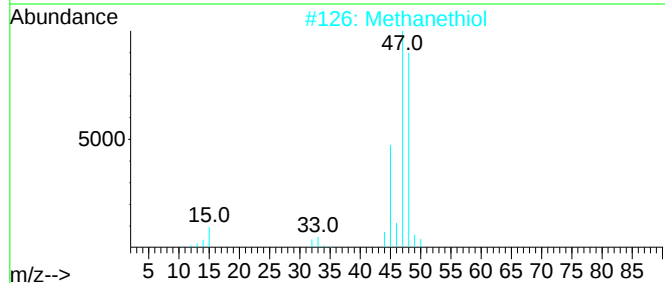
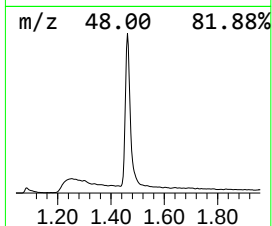
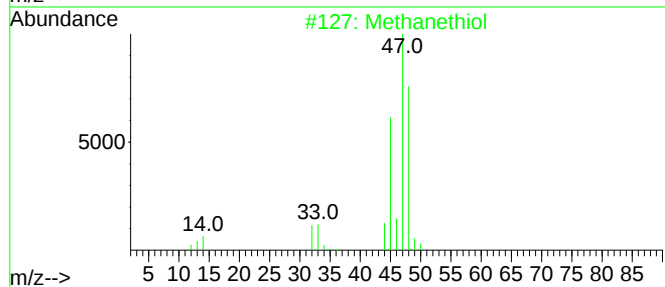
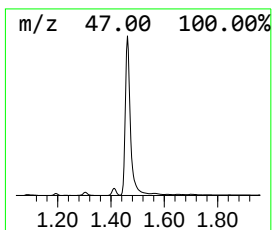
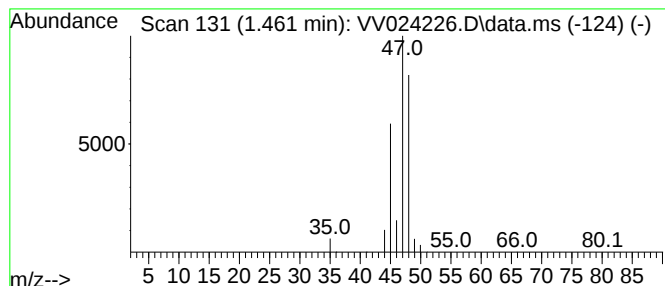
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR122721WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.461	13.08 ug/L	482685	1,4-Difluorobenzene	5.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	91
2			Methanethiol	48	CH4S	000074-93-1	83
3			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4			Methane, nitroso-	45	CH3NO	000865-40-7	5
5			Ethanol	46	C2H6O	000064-17-5	4



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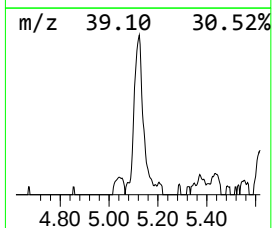
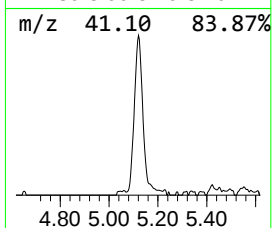
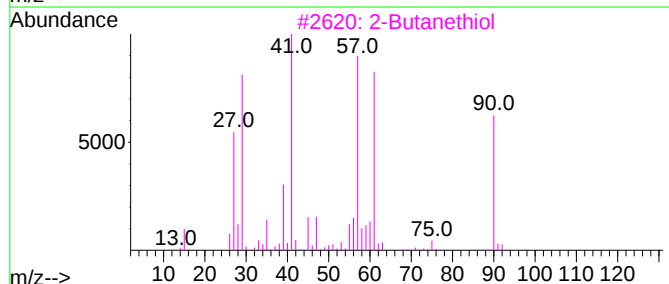
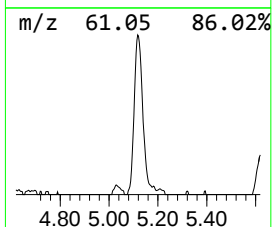
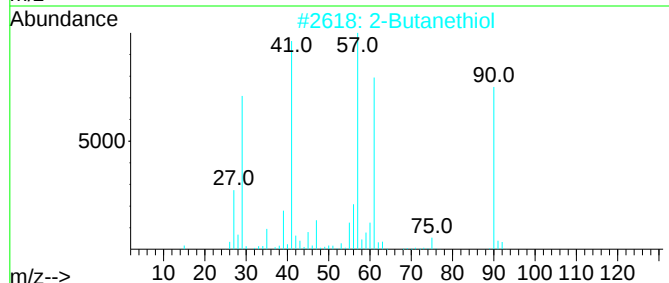
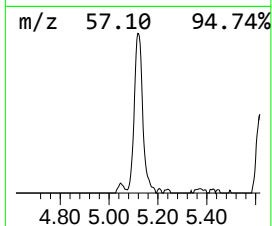
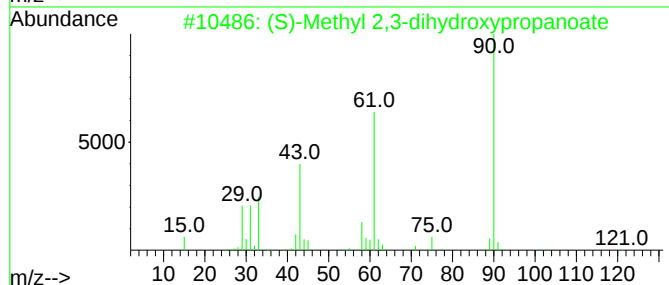
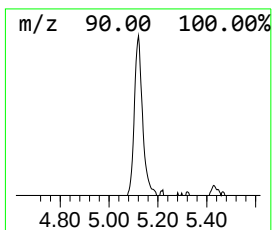
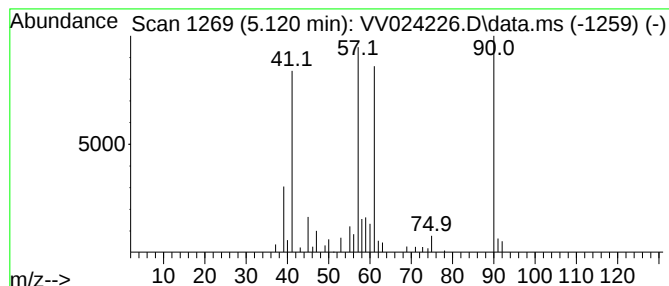
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (S)-Methyl 2,3-dihydroxypro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.120	2.70 ug/L	99612	1,4-Difluorobenzene	5.616

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		(S)-Methyl 2,3-dihydroxypropanoate	120	C4H8O4	010303-88-5	78
2		2-Butanethiol	90	C4H10S	000513-53-1	78
3		2-Butanethiol	90	C4H10S	000513-53-1	74
4		2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	59
5		Thiourea, methyl-	90	C2H6N2S	000598-52-7	42



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Quant Title : TRACE VOA SFAM1.0

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.461	13.1	ug/L	482685	1	5.616	184459	5.0
(S)-Methyl 2,3-...	5.120	2.7	ug/L	99612	1	5.616	184459	5.0