

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
 Data File : VV026560.D
 Acq On : 24 Jun 2022 17:04
 Operator : SY/MD
 Sample : N3425-15
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 COAL8

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\SFAMVTR062322WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV026560.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.256	54	67	80	rBV	18291	61584	9.46%	1.044%
2	1.320	81	87	106	rVB	103668	124272	19.10%	2.106%
3	1.462	116	131	161	rBV2	70389	312884	48.08%	5.303%
4	1.584	162	169	184	rVB	94855	120320	18.49%	2.039%
5	2.121	327	336	352	rVB	179602	263135	40.44%	4.460%
6	2.198	352	360	377	rVB2	6547	16104	2.47%	0.273%
7	2.311	386	395	401	rBV2	4861	7357	1.13%	0.125%
8	2.976	590	602	620	rBV3	4479	10934	1.68%	0.185%
9	3.909	882	892	934	rBV2	55445	184493	28.35%	3.127%
10	4.098	941	951	977	rBV2	29689	81113	12.47%	1.375%
11	4.362	1016	1033	1060	rBV	119912	305451	46.94%	5.177%
12	5.060	1234	1250	1283	rBV2	260820	650695	100.00%	11.028%
13	5.626	1415	1426	1456	rBV	249768	507241	77.95%	8.597%
14	6.079	1553	1567	1591	rBV	147589	306498	47.10%	5.194%
15	6.584	1709	1724	1741	rBV4	24302	56335	8.66%	0.955%
16	6.992	1840	1851	1881	rBV	55198	106616	16.38%	1.807%
17	7.143	1885	1898	1916	rVB3	25881	51808	7.96%	0.878%
18	7.320	1942	1953	1970	rBV	308194	538785	82.80%	9.131%
19	7.397	1971	1977	1990	rVB	12042	24590	3.78%	0.417%
20	7.629	2038	2049	2065	rBV	29465	54713	8.41%	0.927%
21	8.092	2184	2193	2225	rBV	216799	423875	65.14%	7.184%
22	8.854	2416	2430	2455	rBV	365945	597300	91.79%	10.123%
23	9.140	2507	2519	2540	rVB6	7678	18344	2.82%	0.311%
24	10.217	2843	2854	2871	rBV2	99323	156449	24.04%	2.651%
25	11.249	3164	3175	3193	rBV	331579	507598	78.01%	8.603%
26	11.622	3280	3291	3317	rBV	254401	405141	62.26%	6.866%
27	16.484	4796	4803	4812	rVB6	4396	6822	1.05%	0.116%

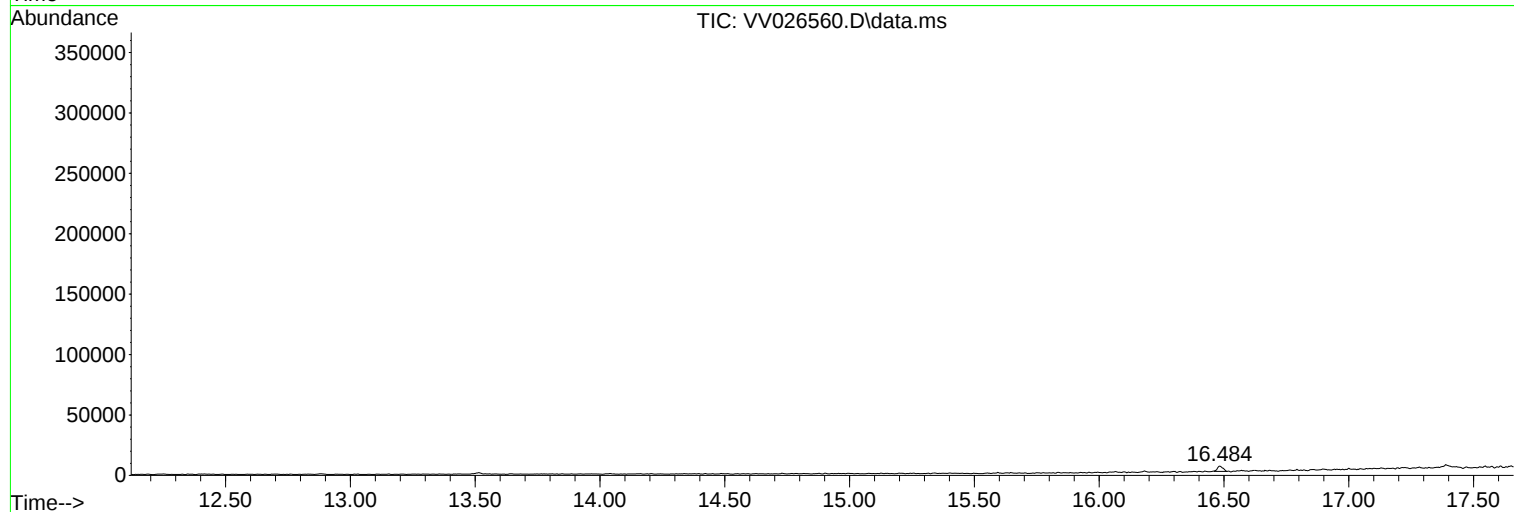
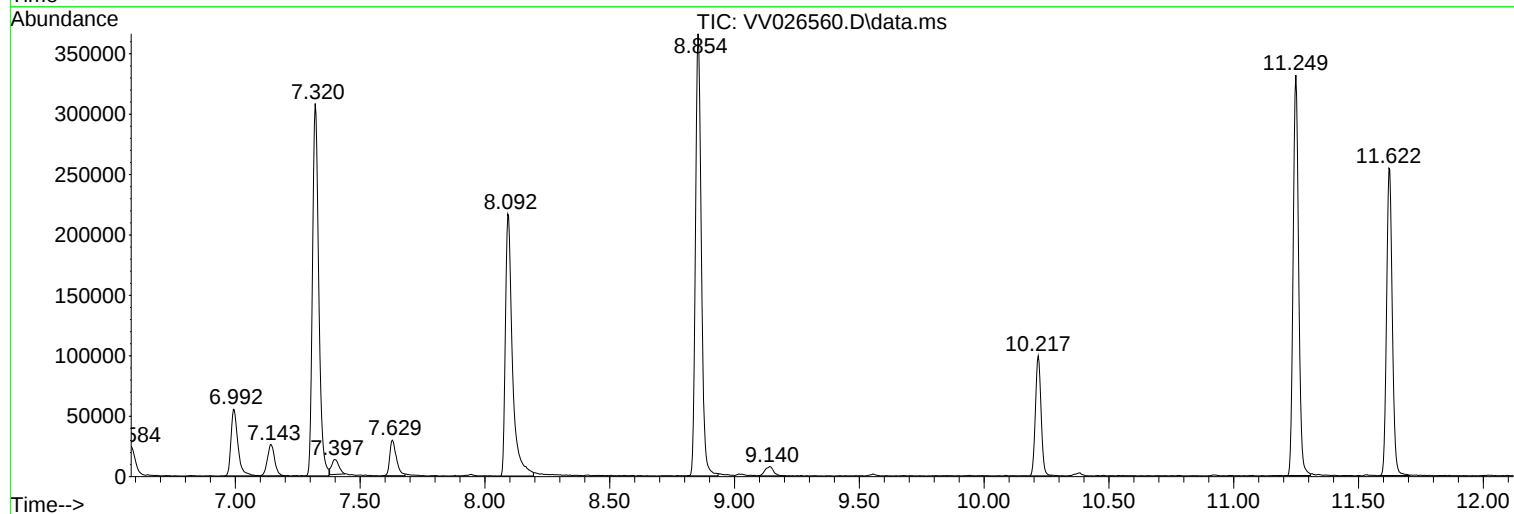
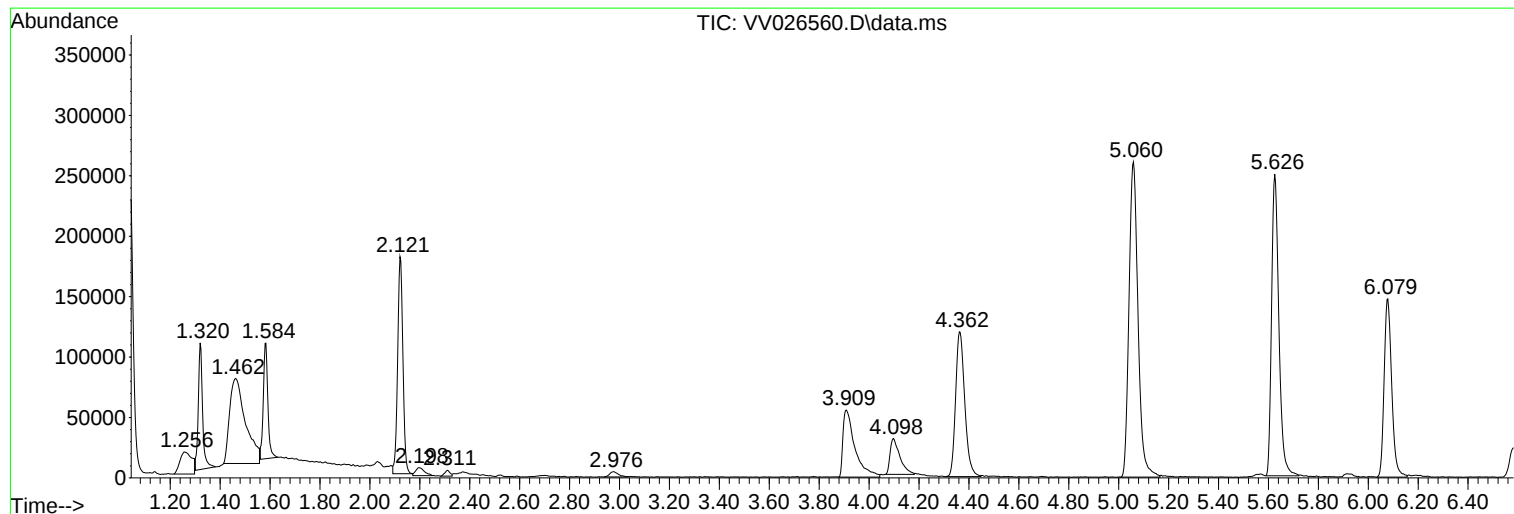
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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
COAL8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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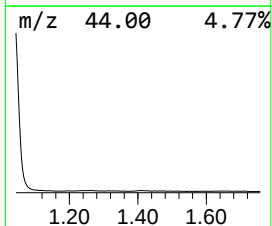
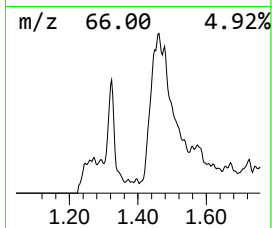
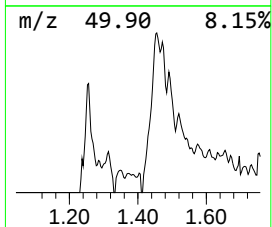
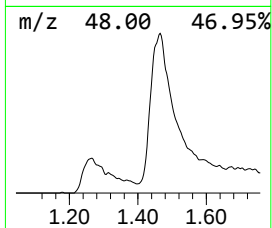
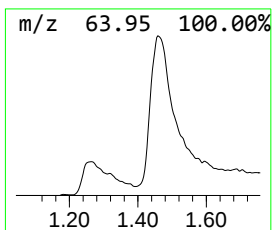
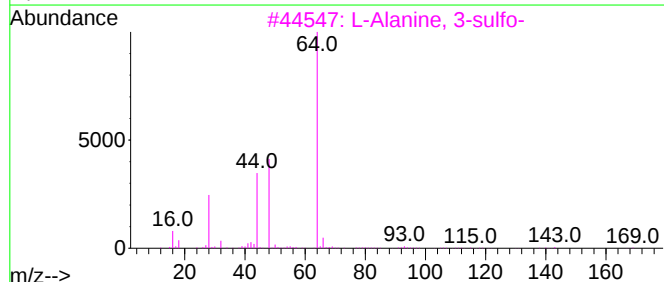
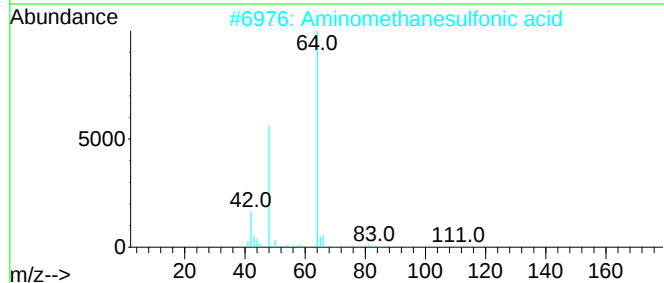
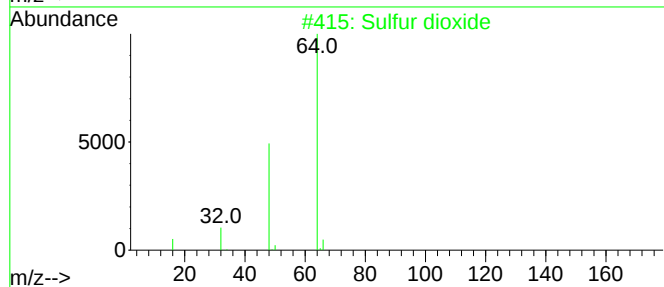
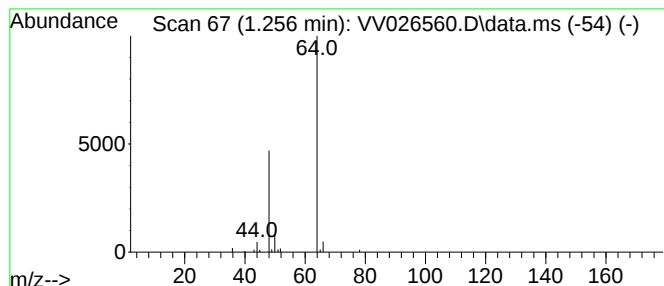
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.256	0.61 ug/L	61584	1,4-Difluorobenzene	5.626

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



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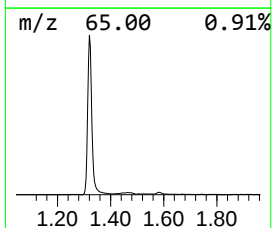
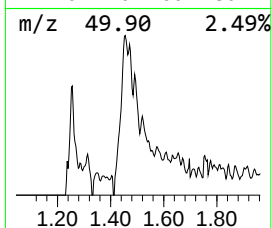
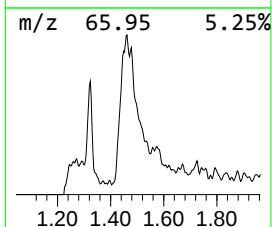
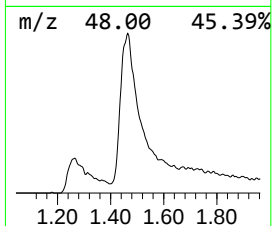
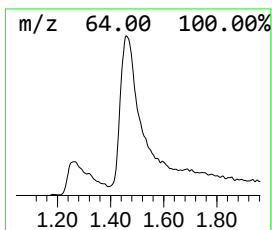
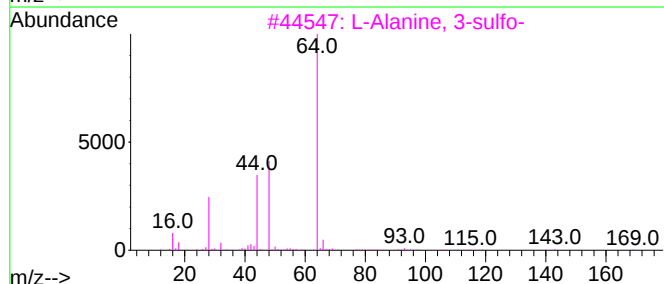
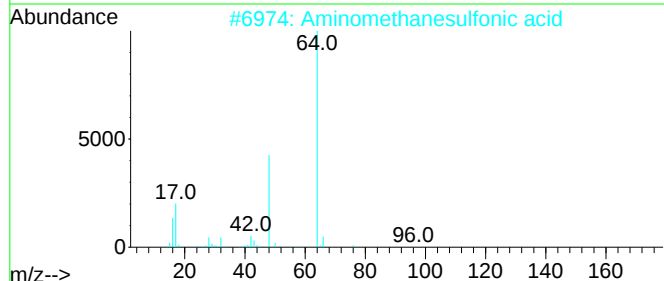
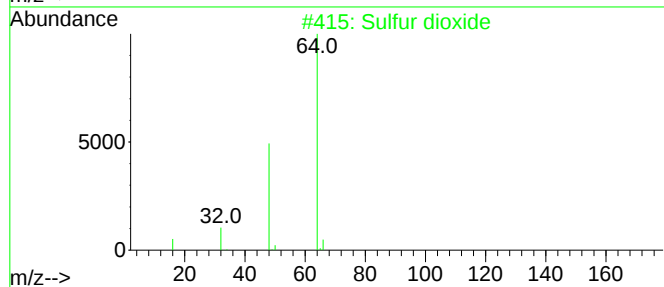
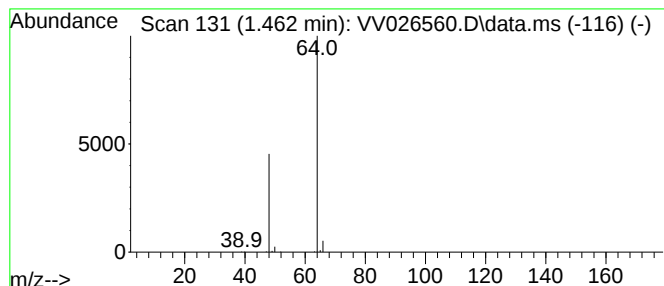
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.462	3.08 ug/L	312884	1,4-Difluorobenzene	5.626

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			Sulfur dioxide	64	O2S	007446-09-5	5



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ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
COAL8

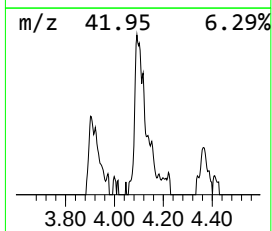
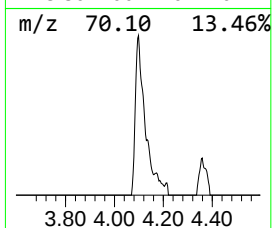
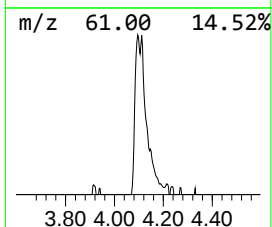
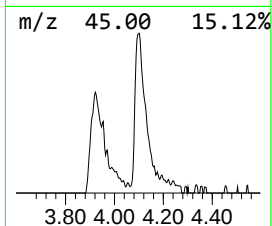
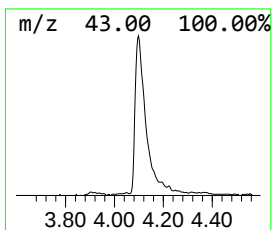
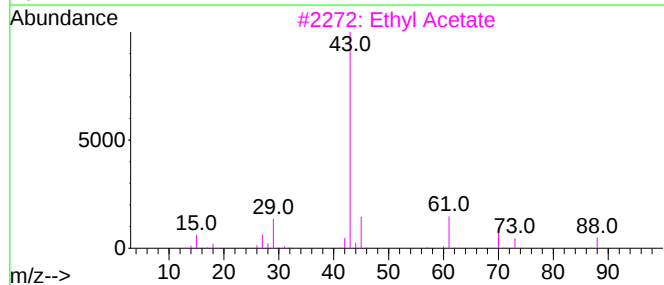
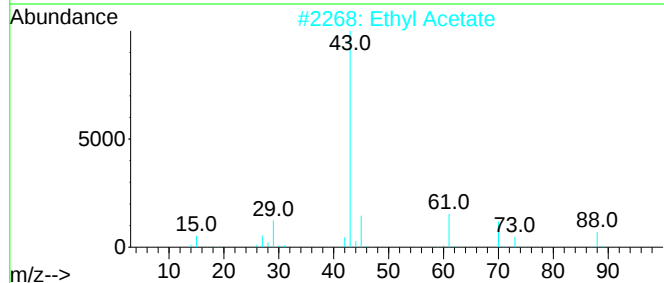
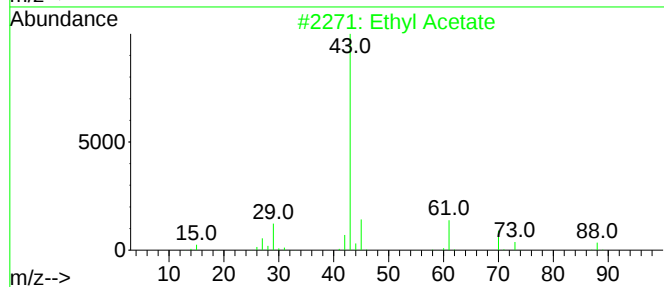
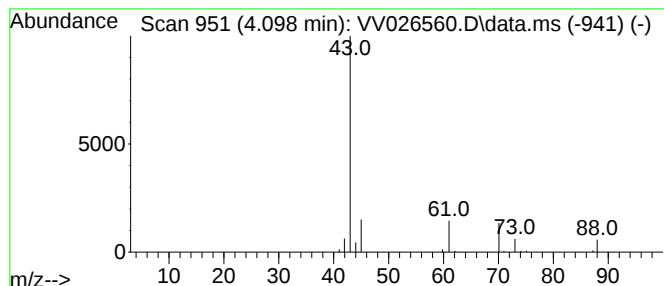
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.098	0.80 ug/L	81113	1,4-Difluorobenzene	5.626

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	86
4			Ethyl Acetate	88	C4H8O2	000141-78-6	78
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	64



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Data File : VV026560.D
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Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
COAL8

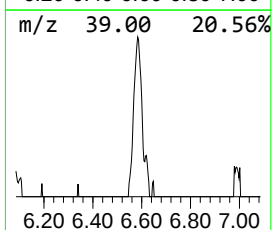
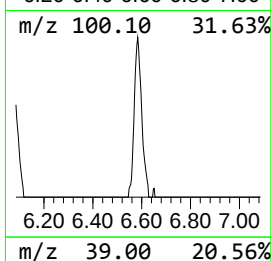
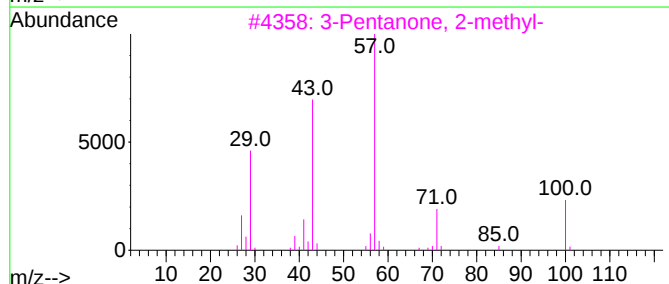
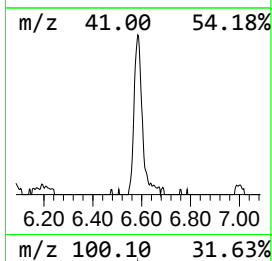
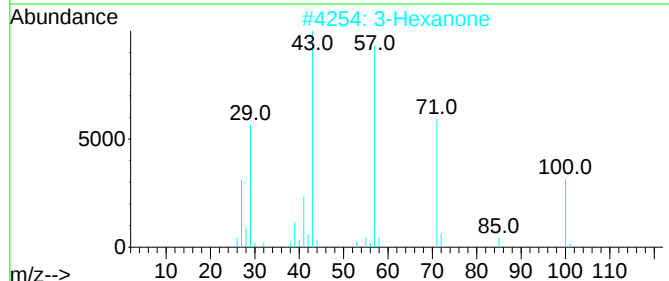
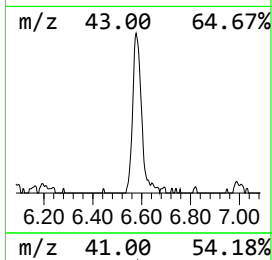
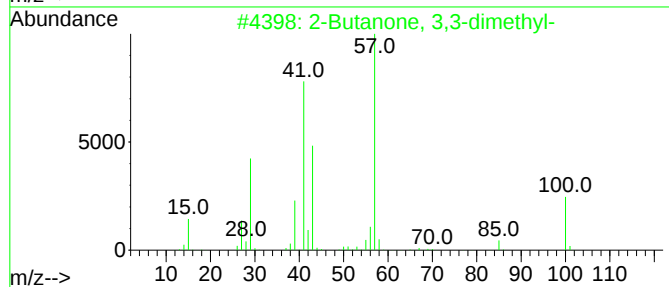
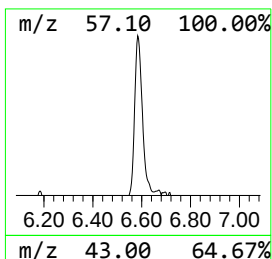
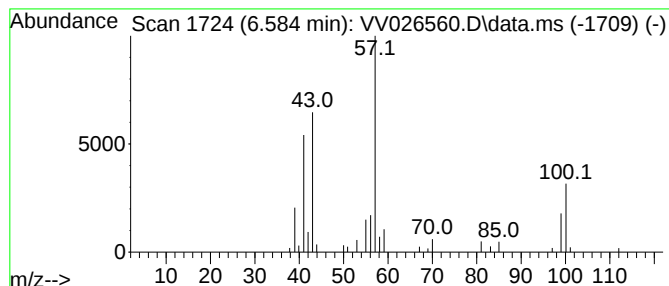
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Butanone, 3,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.584	0.56 ug/L	56335	1,4-Difluorobenzene	5.626

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	53
2	3-Hexanone			100	C6H12O	000589-38-8	50
3	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	49
4	Methyl methacrylate			100	C5H8O2	000080-62-6	47
5	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	46



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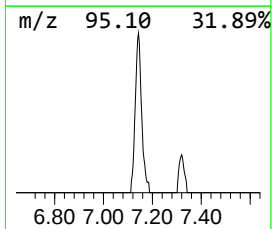
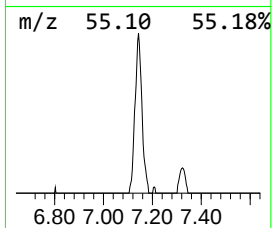
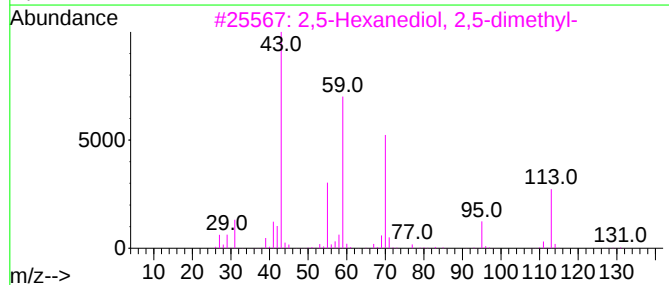
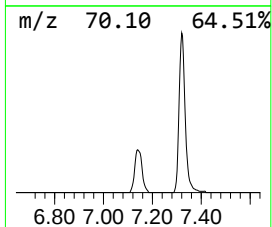
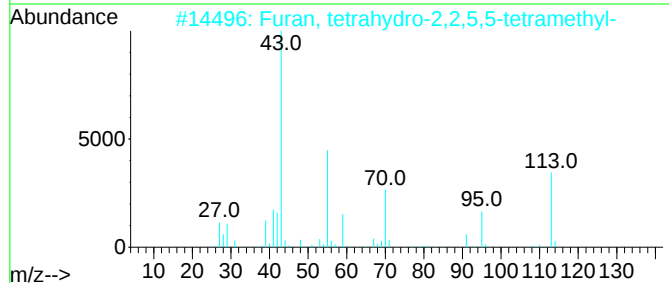
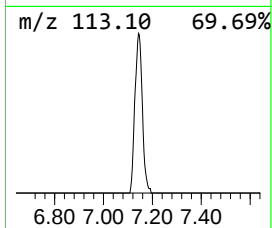
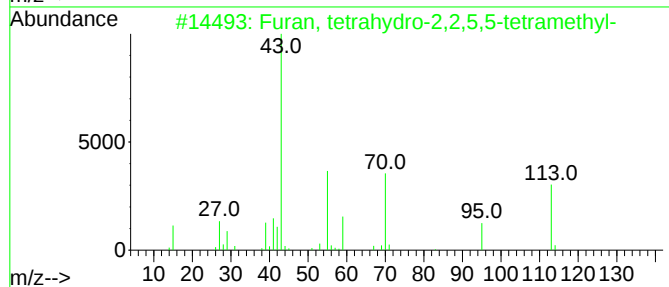
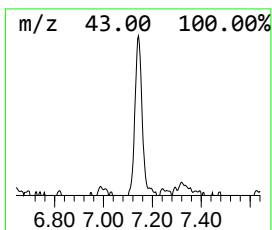
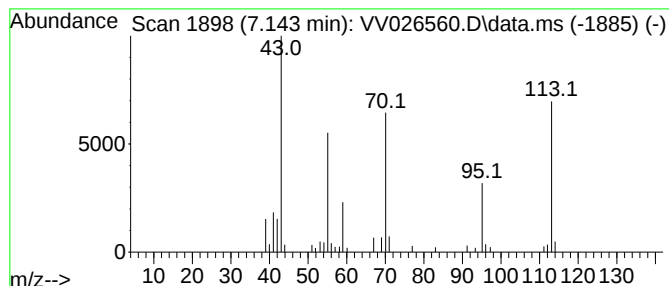
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.143	0.51 ug/L	51808	1,4-Difluorobenzene	5.626

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
3			2,5-Hexanediol, 2,5-dimethyl-	146	C8H18O2	000110-03-2	59
4			Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	59
5			4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.256	0.6	ug/L	61584	1	5.626	507241	5.0
Aminomethanesul...	1.462	3.1	ug/L	312884	1	5.626	507241	5.0
Ethyl Acetate	4.098	0.8	ug/L	81113	1	5.626	507241	5.0
2-Butanone, 3,3...	6.584	0.6	ug/L	56335	1	5.626	507241	5.0
Furan, tetrahyd...	7.143	0.5	ug/L	51808	1	5.626	507241	5.0