

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011323\
 Data File : VV029820.D
 Acq On : 13 Jan 2023 19:51
 Operator : SY/MD
 Sample : 01138-20
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH1Y3

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\SFAMVTR011223WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV029820.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	9	18	36	rVB2	1041344	1794998	7.72%	3.986%
2	1.455	122	129	154	rBV	371594	562326	2.42%	1.249%
3	2.021	296	305	320	rBV	652110	995368	4.28%	2.210%
4	2.105	321	331	357	rVV3	783252	1327029	5.71%	2.947%
5	2.278	369	385	404	rBV2	439588	2189915	9.42%	4.863%
6	2.388	407	419	450	rVB	975955	3962678	17.04%	8.799%
7	3.175	657	664	695	rVB	142102	321171	1.38%	0.713%
8	3.895	874	888	910	rVB	674890	1596256	6.87%	3.544%
9	4.336	1016	1025	1068	rVB	155181	448523	1.93%	0.996%
10	4.542	1075	1089	1116	rVB	166214	479528	2.06%	1.065%
11	5.030	1226	1241	1260	rBV2	346669	752628	3.24%	1.671%
12	5.603	1401	1419	1437	rBV	256471	506721	2.18%	1.125%
13	5.892	1491	1509	1527	rBV	12508338	23252033	100.00%	51.629%
14	5.982	1530	1537	1550	rVV4	101726	252279	1.08%	0.560%
15	6.056	1551	1560	1571	rVB	157302	286492	1.23%	0.636%
16	6.185	1580	1600	1610	rBV3	109964	403173	1.73%	0.895%
17	6.374	1648	1659	1674	rVB	766212	1400831	6.02%	3.110%
18	7.291	1932	1944	1958	rBV	385863	650804	2.80%	1.445%
19	7.600	2024	2040	2053	rBV3	286776	674367	2.90%	1.497%
20	8.040	2168	2177	2189	rBV	460676	714885	3.07%	1.587%
21	8.108	2190	2198	2216	rVV	297409	541978	2.33%	1.203%
22	8.837	2414	2425	2433	rBV	338150	532241	2.29%	1.182%
23	10.207	2835	2851	2865	rBV	138187	263342	1.13%	0.585%
24	11.236	3158	3171	3189	rBV	367912	581470	2.50%	1.291%
25	11.612	3276	3288	3303	rBV	346734	545309	2.35%	1.211%

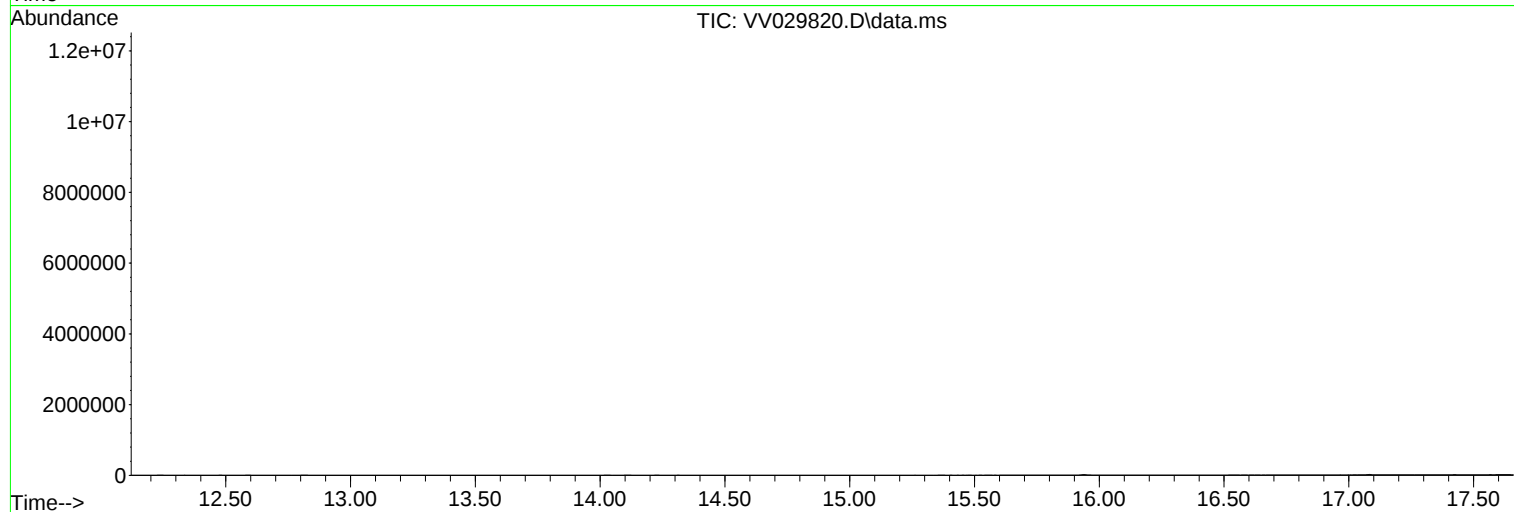
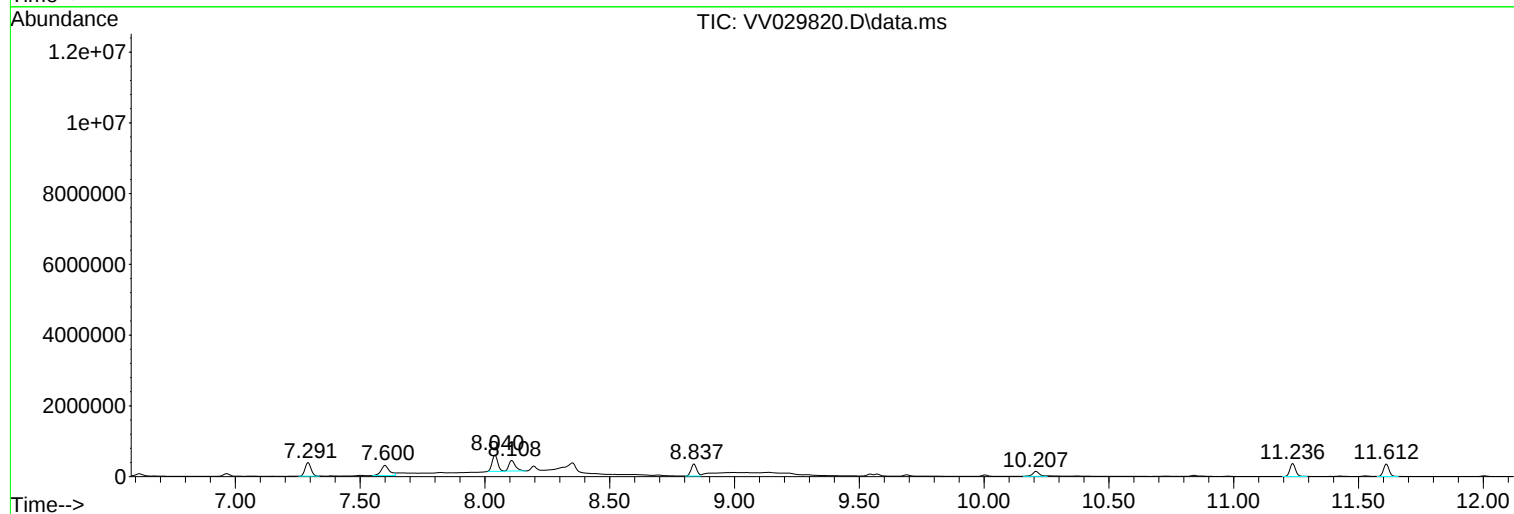
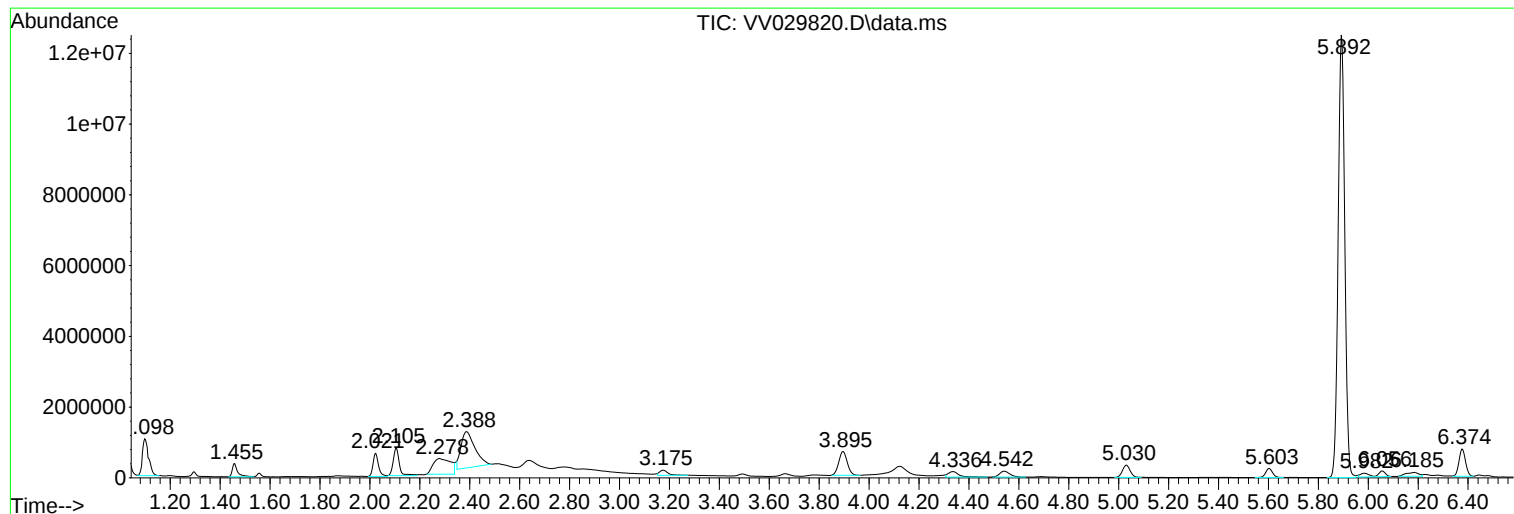
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011223WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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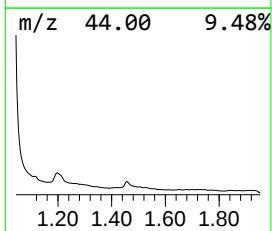
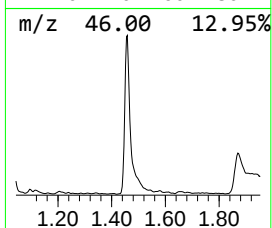
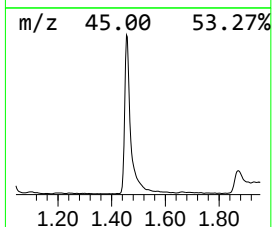
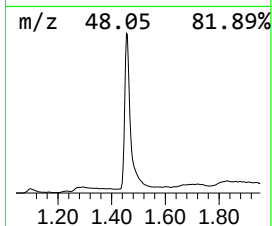
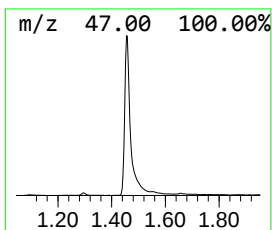
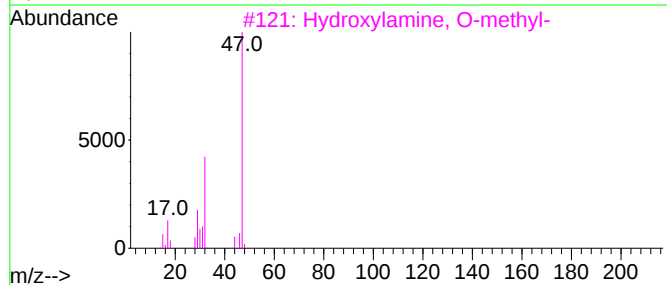
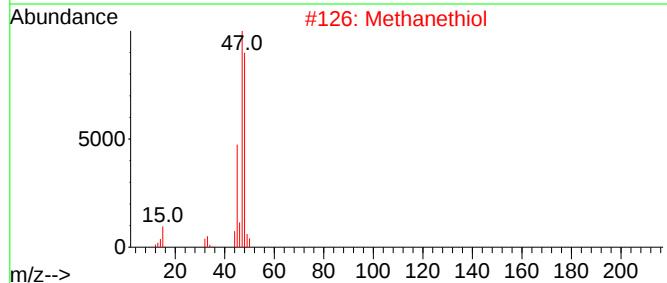
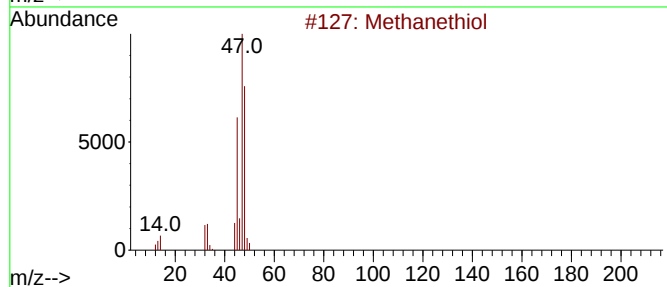
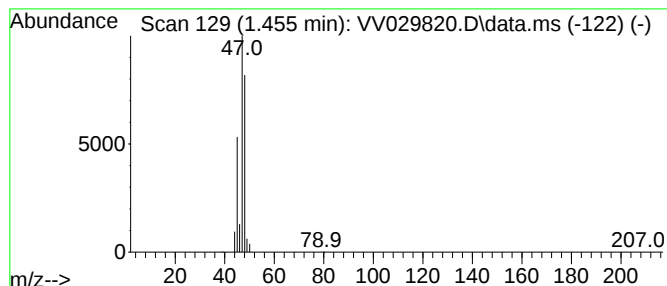
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Methanethiol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.455	5.55 ug/L	562326	1,4-Difluorobenzene	5.603

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	91
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			Methane, nitroso-	45	CH3NO	000865-40-7	5



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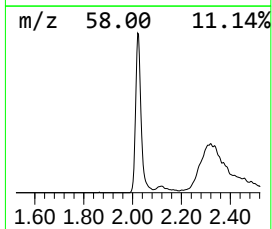
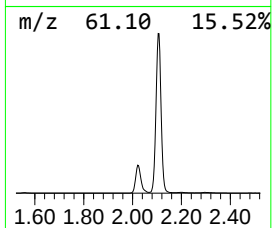
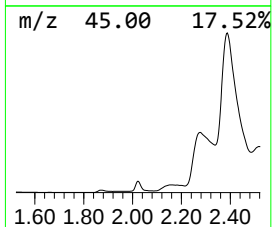
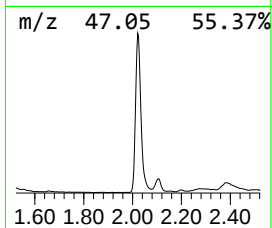
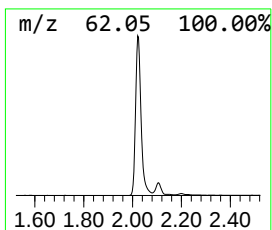
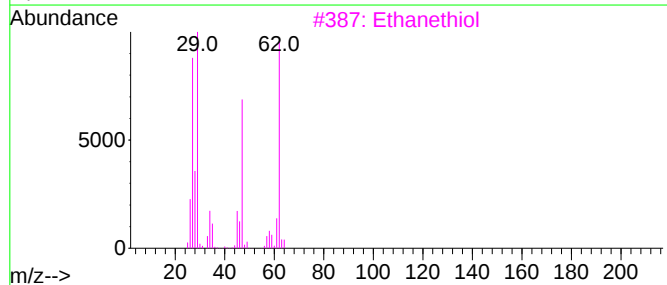
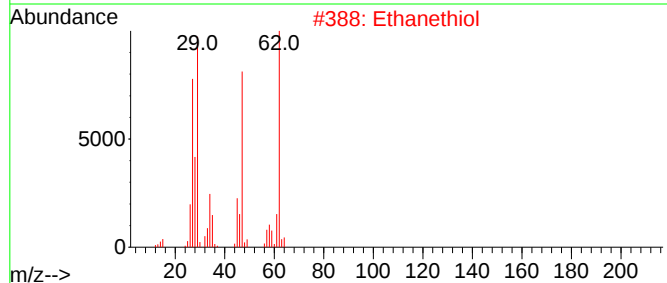
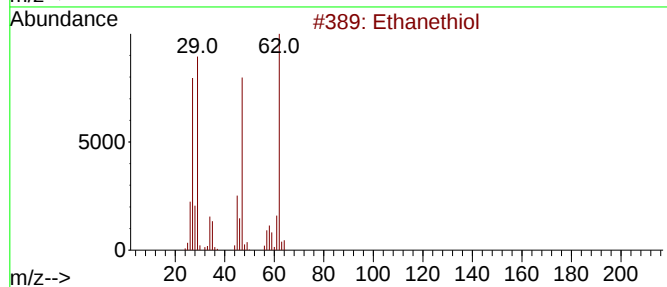
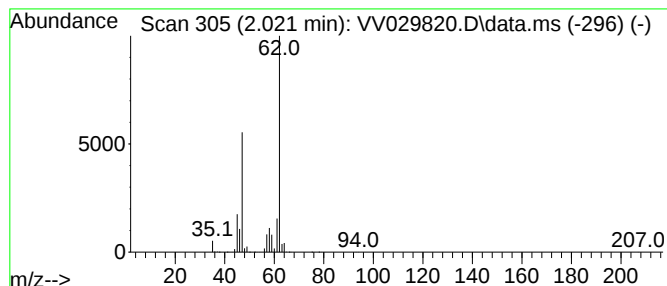
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Ethanethiol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.021	9.82 ug/L	995368	1,4-Difluorobenzene	5.603

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



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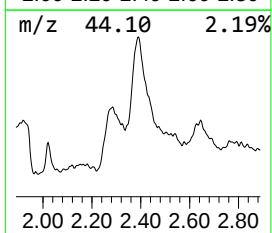
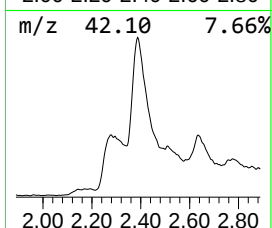
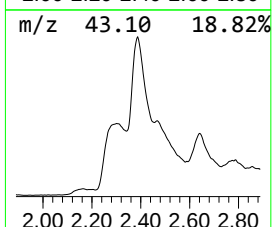
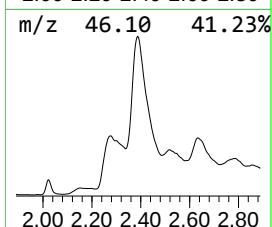
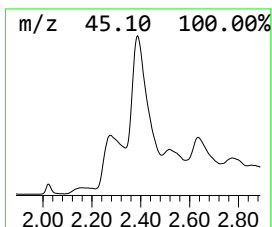
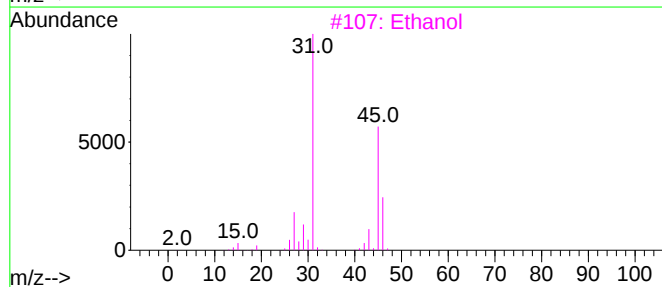
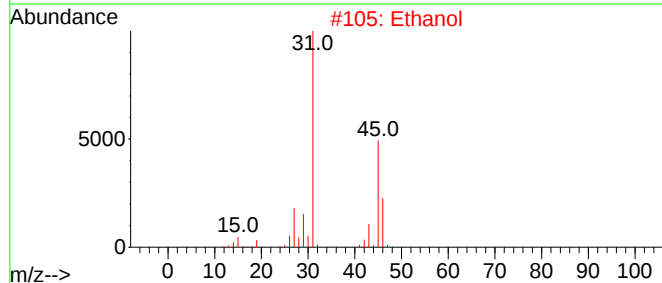
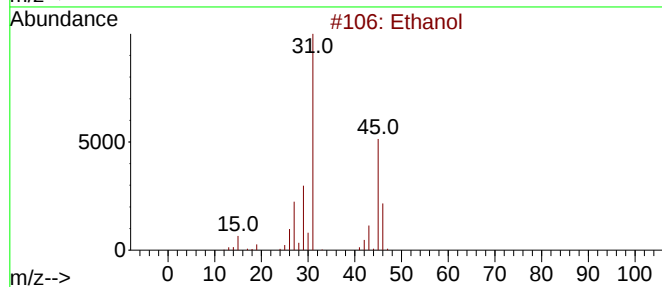
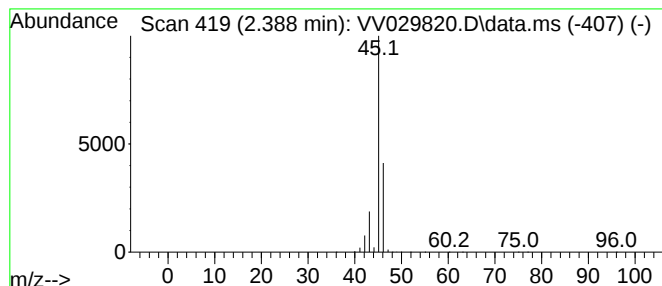
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011223WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.388	39.10 ug/L	3962680	1,4-Difluorobenzene	5.603

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	86
2	Ethanol			46	C2H6O	000064-17-5	78
3	Ethanol			46	C2H6O	000064-17-5	78
4	Dimethyl ether			46	C2H6O	000115-10-6	9
5	Dimethyl ether			46	C2H6O	000115-10-6	9



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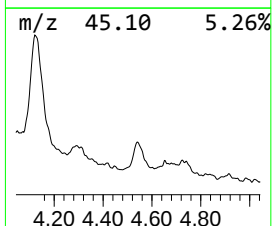
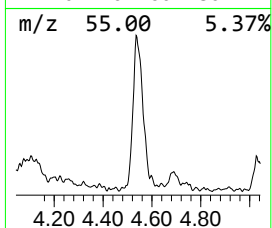
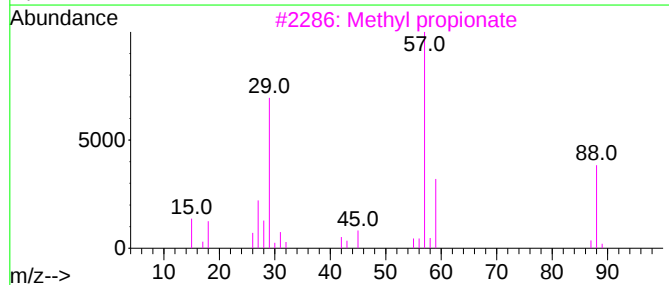
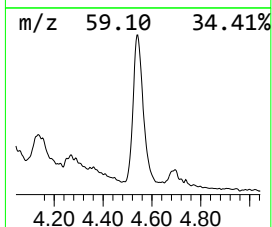
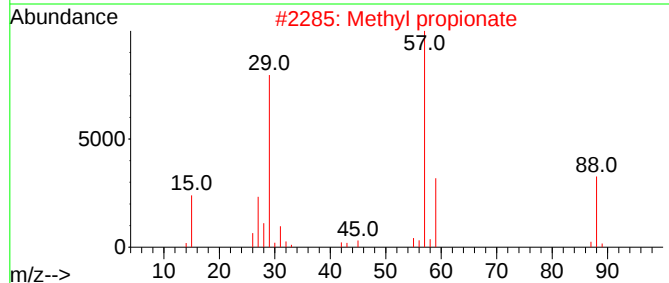
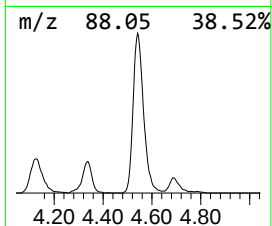
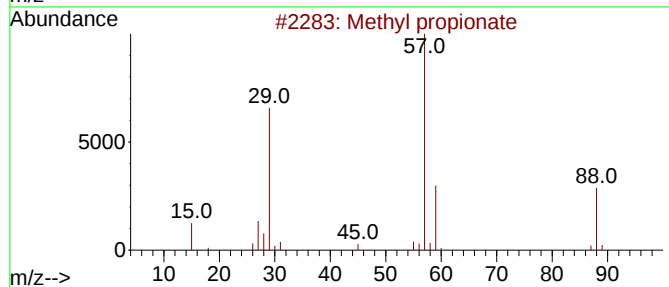
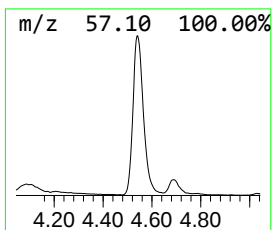
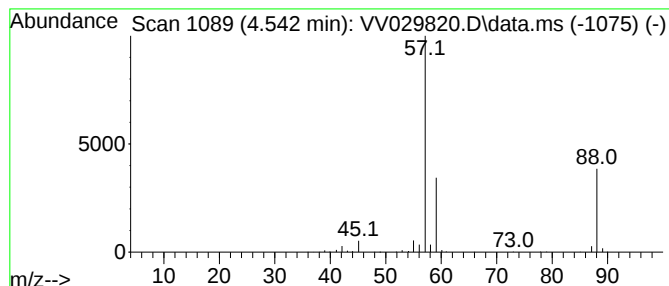
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Methyl propionate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.542	4.73 ug/L	479528	1,4-Difluorobenzene	5.603

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl propionate			88	C4H8O2	000554-12-1	90
2	Methyl propionate			88	C4H8O2	000554-12-1	86
3	Methyl propionate			88	C4H8O2	000554-12-1	83
4	Methyl propionate			88	C4H8O2	000554-12-1	80
5	Methyl propionate			88	C4H8O2	000554-12-1	64



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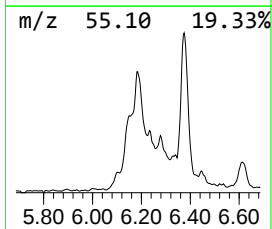
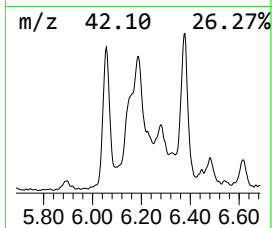
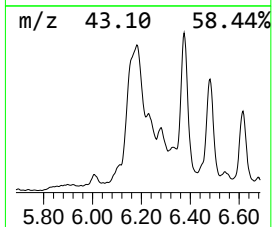
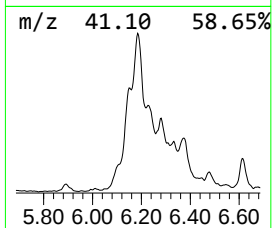
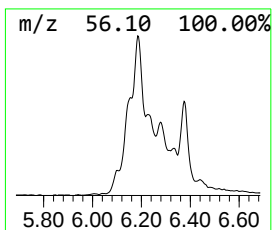
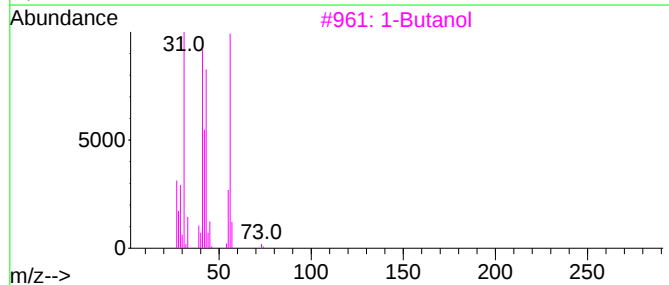
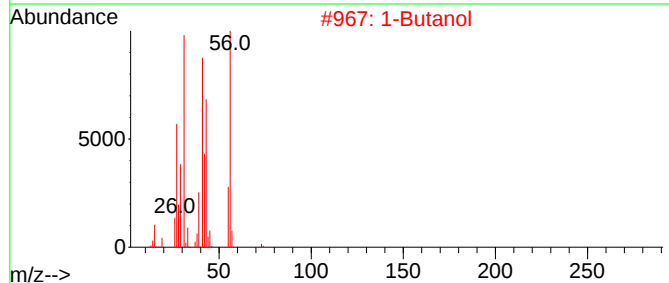
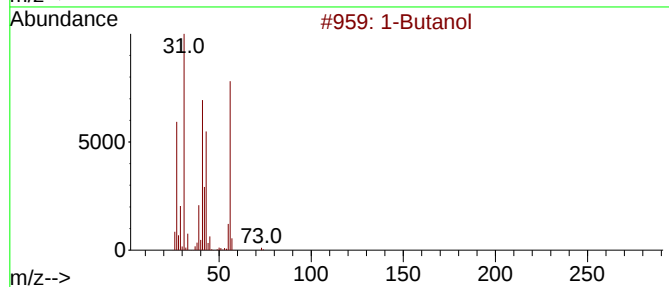
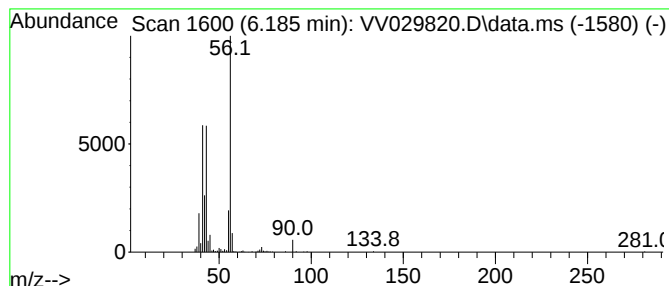
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.185	3.98 ug/L	403173	1,4-Difluorobenzene	5.603

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	80
2	1-Butanol		74	C4H10O	000071-36-3	80
3	1-Butanol		74	C4H10O	000071-36-3	80
4	1-Butanol		74	C4H10O	000071-36-3	80
5	1-Butanol		74	C4H10O	000071-36-3	72



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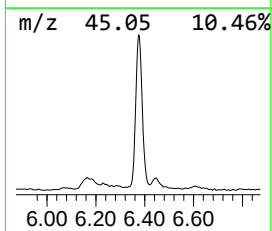
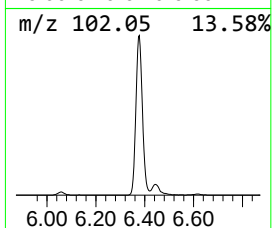
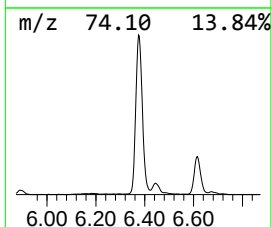
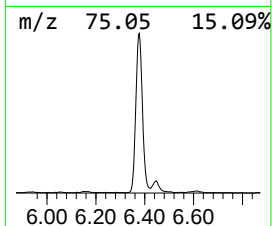
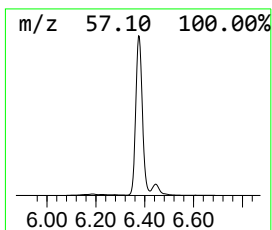
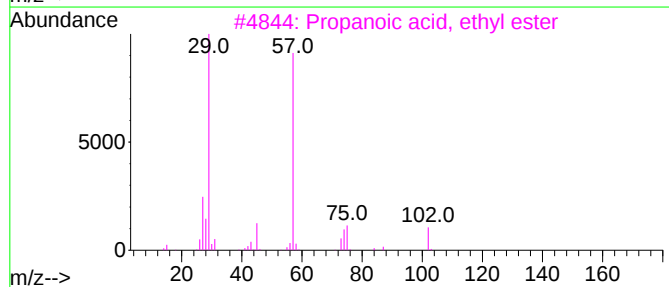
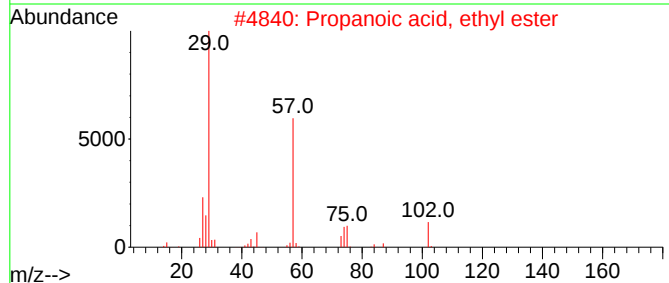
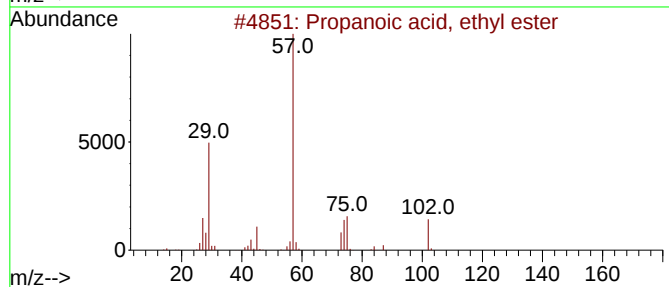
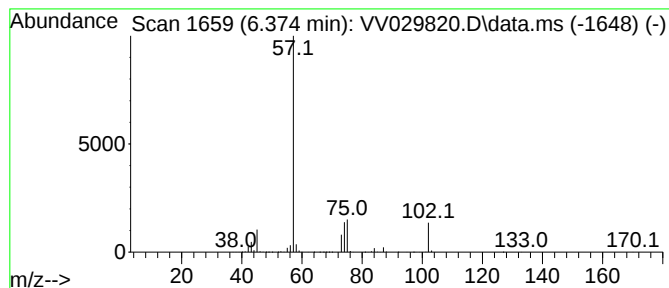
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Propanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.374	13.82 ug/L	1400830	1,4-Difluorobenzene	5.603

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	91
2			Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	90
3			Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	90
4			Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	86
5			Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011323\
Data File : VV029820.D
Acq On : 13 Jan 2023 19:51
Operator : SY/MD
Sample : 01138-20
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH1Y3

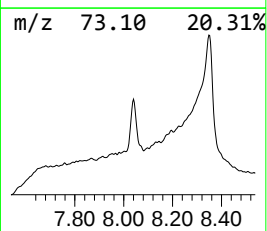
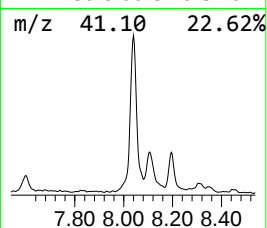
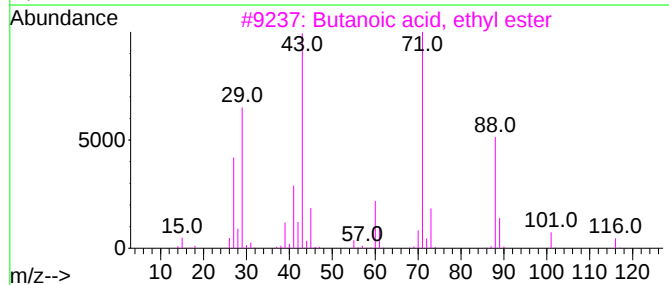
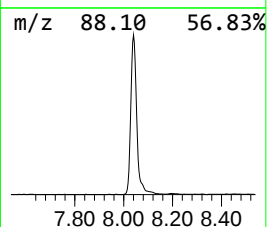
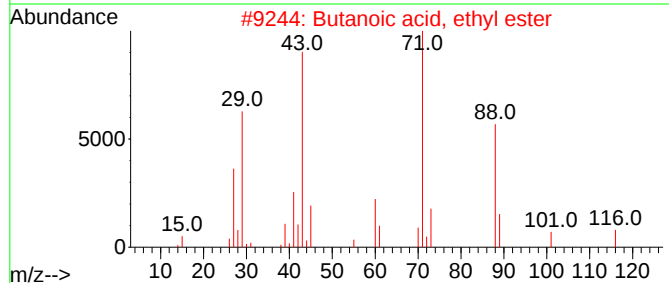
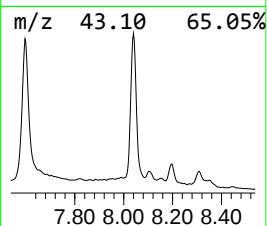
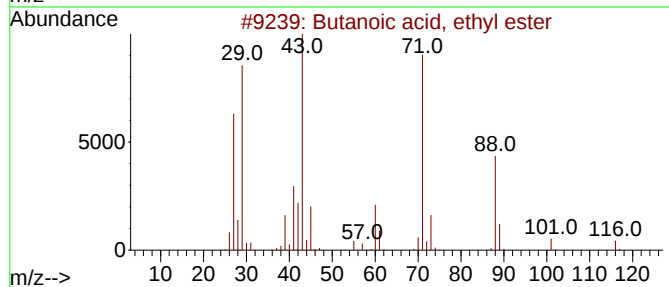
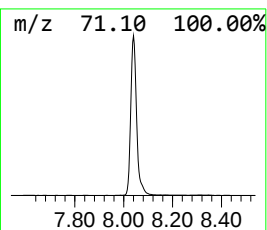
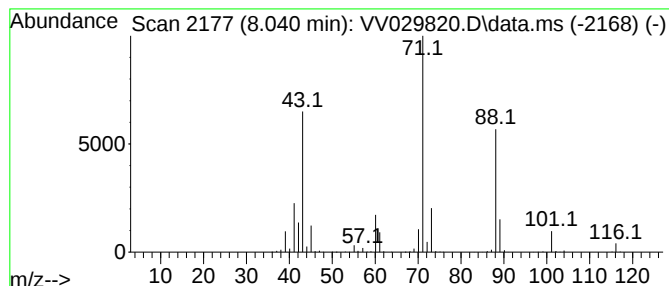
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Butanoic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.040	6.72 ug/L	714885	Chlorobenzene-d5	8.837

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	91
4			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	76
5			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011323\
Data File : VV029820.D
Acq On : 13 Jan 2023 19:51
Operator : SY/MD
Sample : 01138-20
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH1Y3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011223WMA.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
Methanethiol	1.455	5.5	ug/L	562326	1	5.603	506721	5.0
Ethanethiol	2.021	9.8	ug/L	995368	1	5.603	506721	5.0
Ethanol	2.388	39.1	ug/L	3962680	1	5.603	506721	5.0
Methyl propionate	4.542	4.7	ug/L	479528	1	5.603	506721	5.0
1-Butanol	6.185	4.0	ug/L	403173	1	5.603	506721	5.0
Propanoic acid,...	6.374	13.8	ug/L	1400830	1	5.603	506721	5.0
Butanoic acid, ...	8.040	6.7	ug/L	714885	2	8.837	532241	5.0