

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091924\
 Data File : VU060908.D
 Acq On : 19 Sep 2024 19:08
 Operator : MD/SY
 Sample : P3987-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH8P5

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_U\Method\SFAMUTR091624WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU060908.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.377	22	27	34	rVB	33140	34879	1.00%	0.271%
2	1.599	86	96	103	rBV2	87508	134852	3.88%	1.048%
3	1.785	149	154	168	rVB	63346	76716	2.21%	0.596%
4	1.911	187	193	212	rVB	45556	68200	1.96%	0.530%
5	2.467	357	366	381	rBV2	43304	76005	2.19%	0.590%
6	2.573	385	399	410	rVV2	525426	924580	26.61%	7.183%
7	2.641	410	420	454	rVV	284970	708857	20.40%	5.507%
8	2.946	505	515	537	rBV	281366	563202	16.21%	4.376%
9	3.178	574	587	597	rBV	16615	38440	1.11%	0.299%
10	3.358	631	643	657	rBV5	16051	35542	1.02%	0.276%
11	3.859	781	799	830	rBV	578605	1391250	40.04%	10.809%
12	4.657	1018	1047	1088	rBV3	727591	2168221	62.40%	16.845%
13	5.055	1154	1171	1198	rBV2	81934	200724	5.78%	1.559%
14	5.718	1358	1377	1392	rBV2	146199	387993	11.17%	3.014%
15	6.242	1528	1540	1566	rBV2	153248	302874	8.72%	2.353%
16	6.534	1616	1631	1666	rBV	1776263	3474736	100.00%	26.995%
17	6.682	1667	1677	1694	rVB2	92720	184967	5.32%	1.437%
18	7.177	1819	1831	1858	rBV	115785	221828	6.38%	1.723%
19	7.560	1937	1950	1965	rBV2	36072	65701	1.89%	0.510%
20	7.891	2041	2053	2070	rBV	173765	323552	9.31%	2.514%
21	8.177	2129	2142	2160	rBV4	23500	44965	1.29%	0.349%
22	8.627	2272	2282	2318	rBV2	175758	359744	10.35%	2.795%
23	9.412	2511	2526	2558	rBV	218097	386926	11.14%	3.006%
24	10.750	2931	2942	2961	rVB2	70095	115749	3.33%	0.899%
25	11.807	3260	3271	3292	rBV	196738	325457	9.37%	2.528%
26	12.187	3377	3389	3411	rBV	149294	255611	7.36%	1.986%

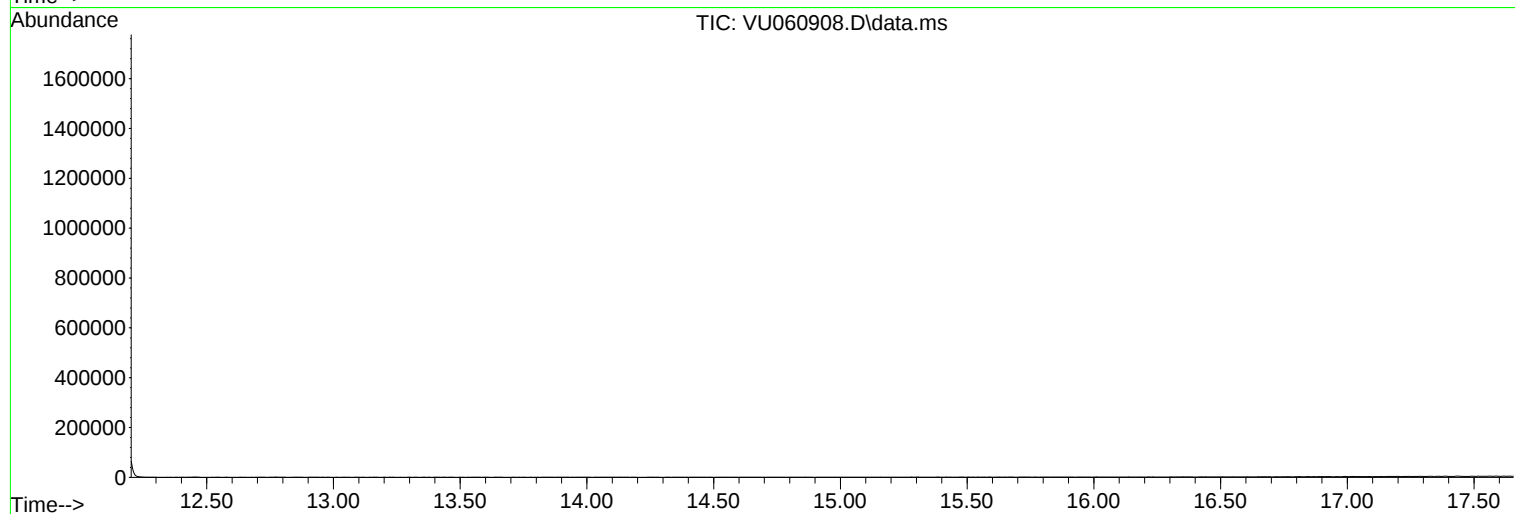
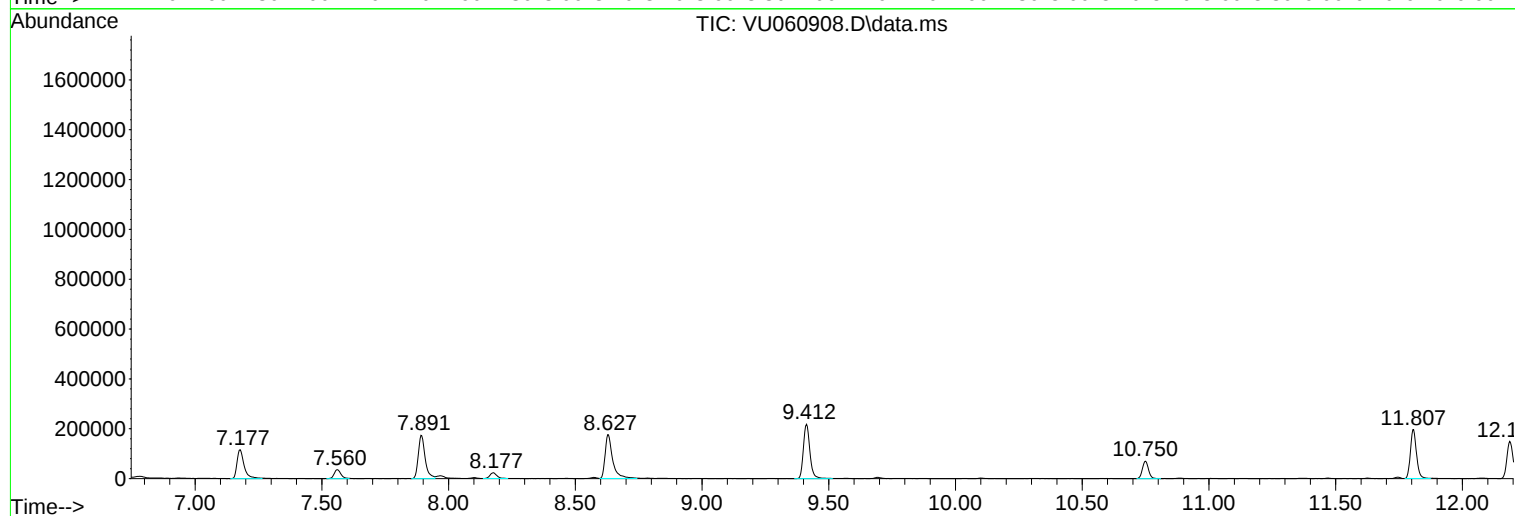
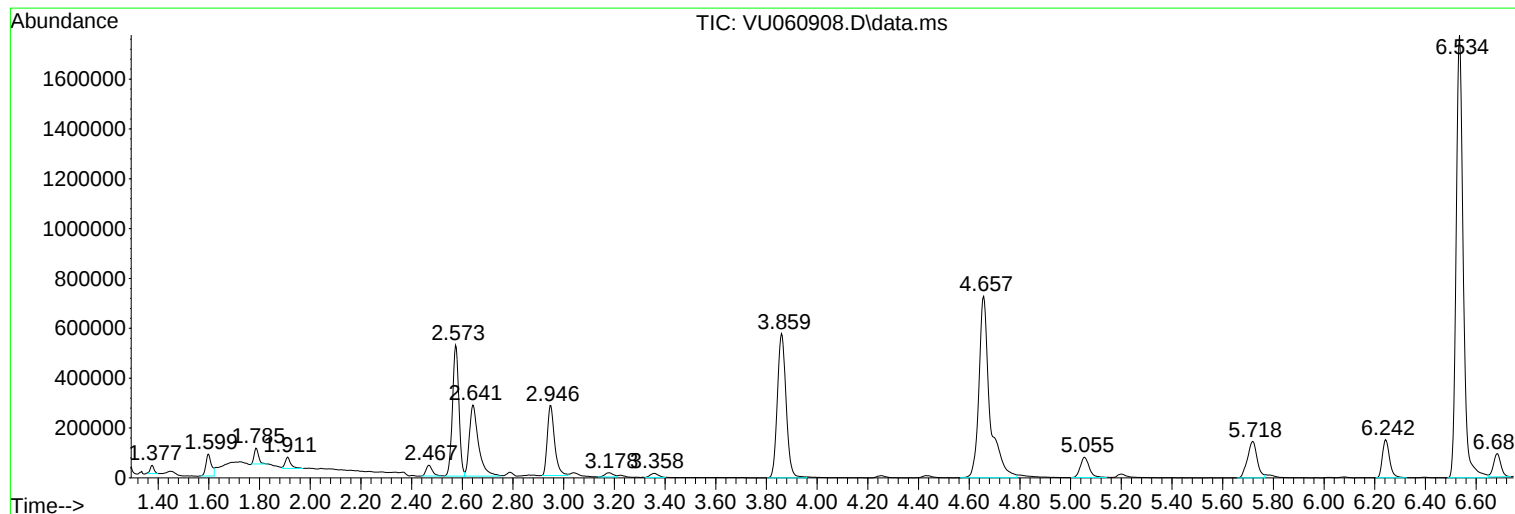
Sum of corrected areas: 12871571

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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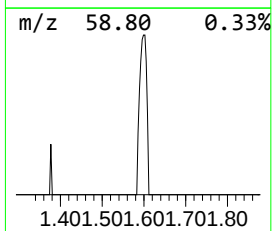
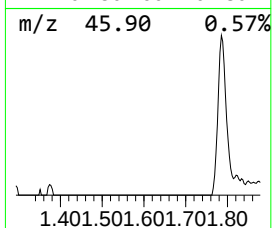
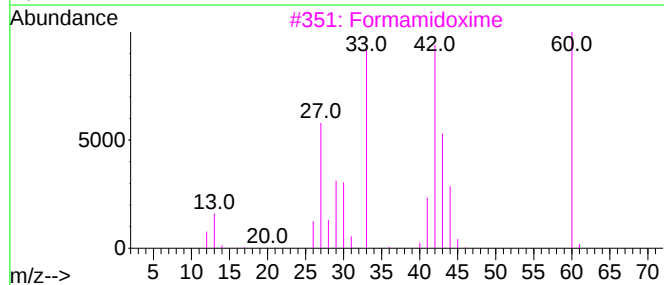
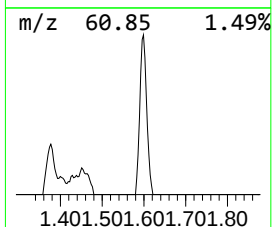
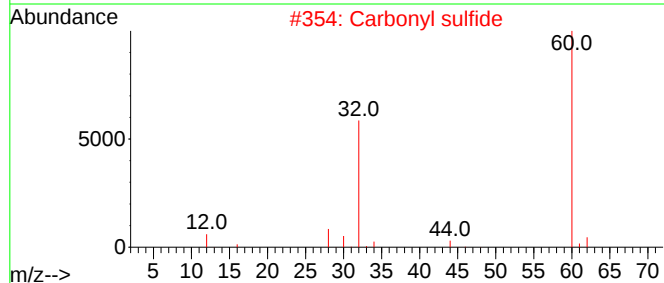
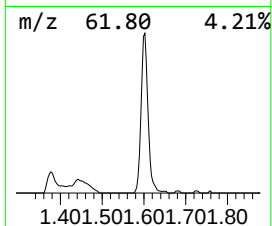
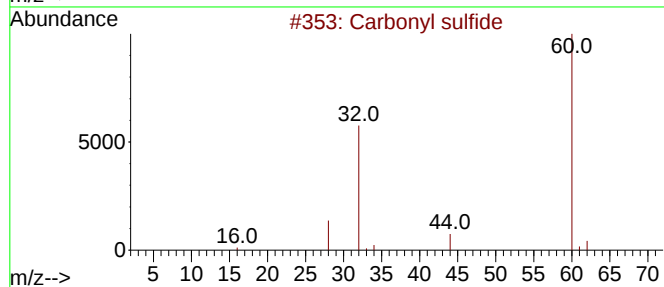
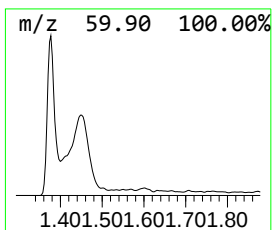
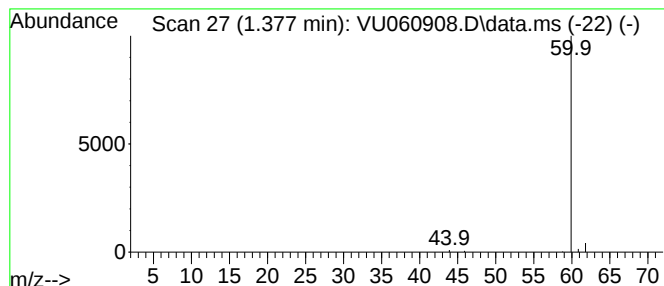
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.377	0.58 ug/L	34879	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonyl sulfide	60	COS	000463-58-1	5
2			Carbonyl sulfide	60	COS	000463-58-1	5
3			Formamidoxime	60	CH4N2O	000624-82-8	5
4			Thiirane	60	C2H4S	000420-12-2	4
5			Urea	60	CH4N2O	000057-13-6	4



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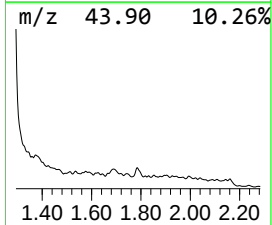
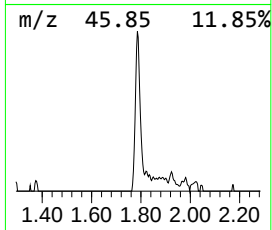
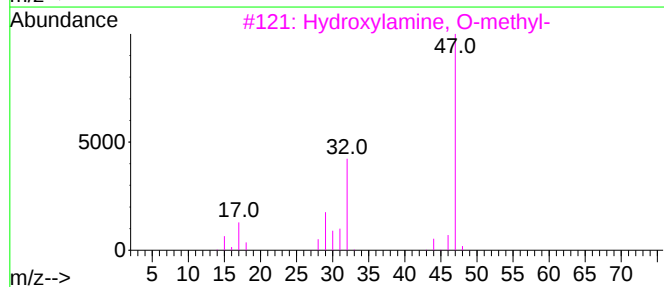
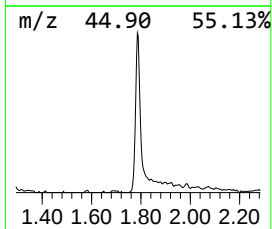
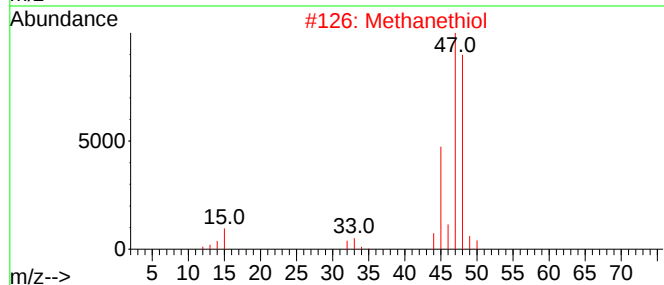
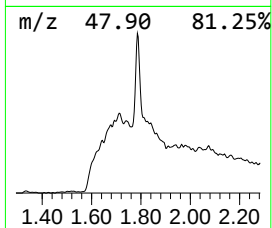
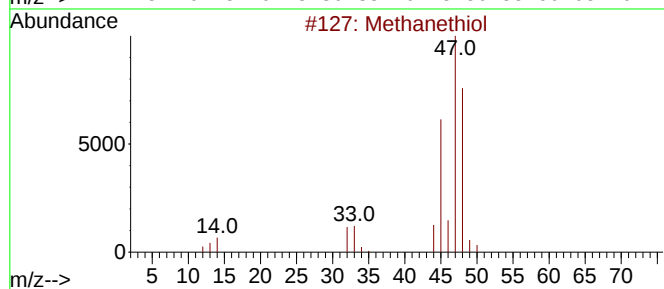
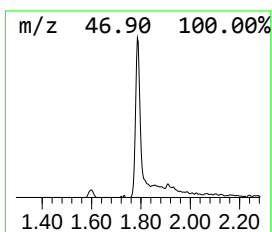
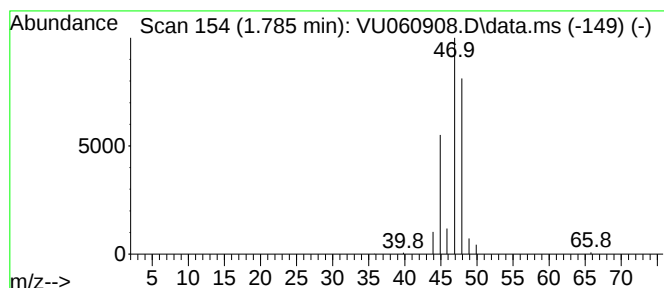
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.785	1.27 ug/L	76716	1,4-Difluorobenzene	6.242

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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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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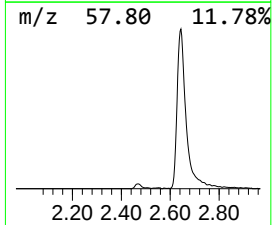
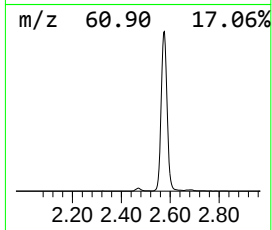
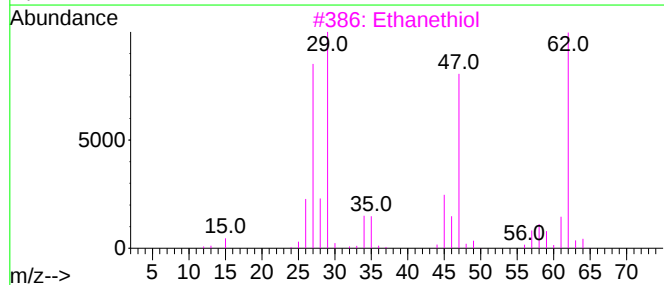
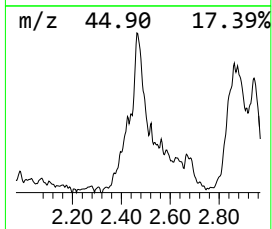
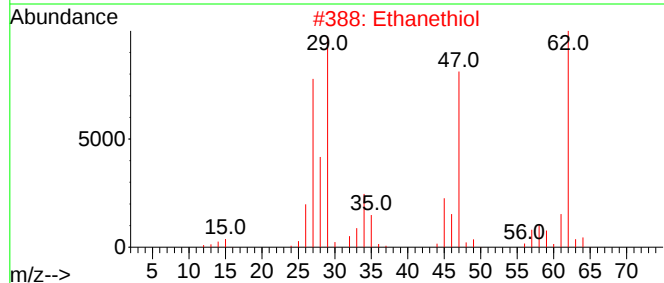
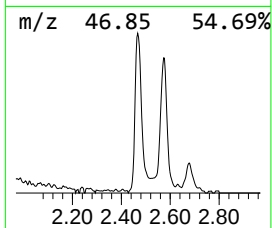
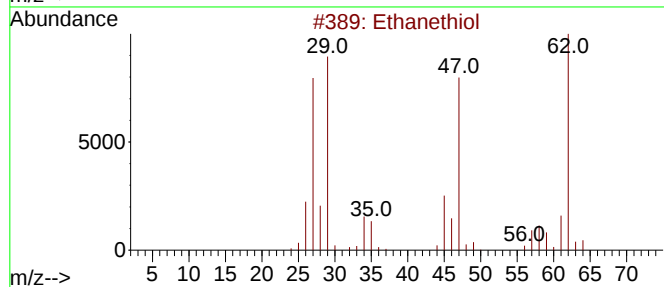
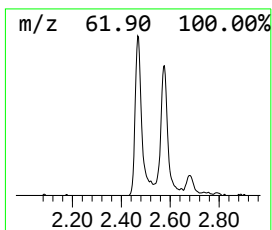
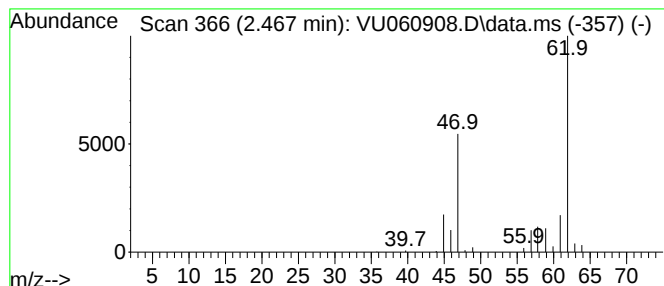
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.467	1.25 ug/L	76005	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol			62	C2H6S	000075-08-1	90
2	Ethanethiol			62	C2H6S	000075-08-1	90
3	Ethanethiol			62	C2H6S	000075-08-1	90
4	Ethanethiol			62	C2H6S	000075-08-1	83
5	Ethanethiol			62	C2H6S	000075-08-1	83



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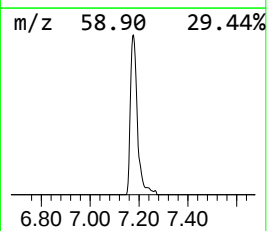
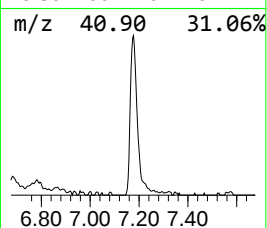
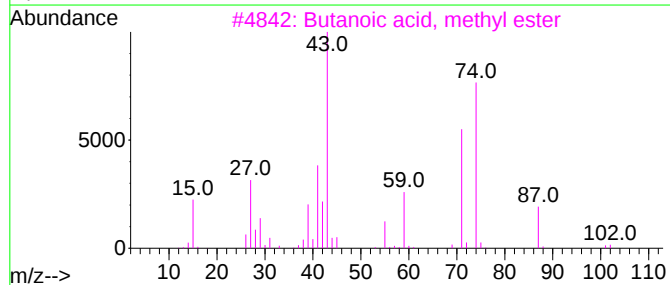
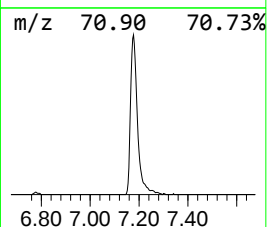
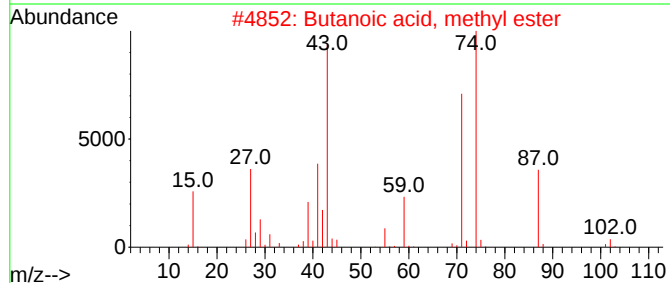
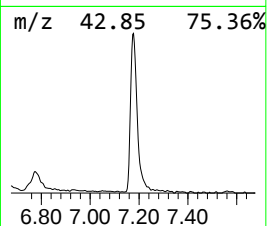
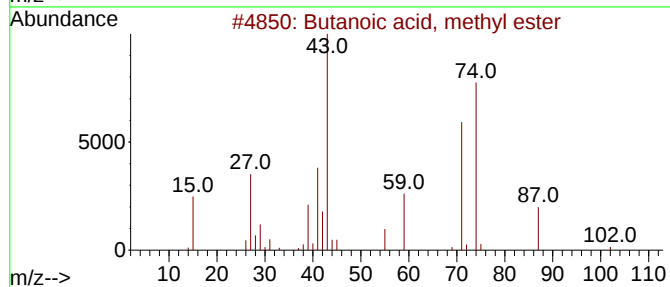
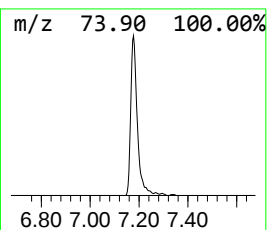
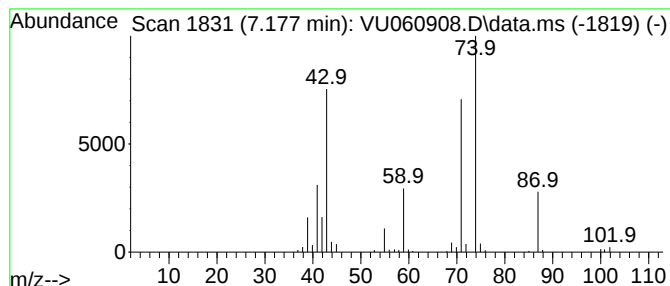
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Butanoic acid, methyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.177	3.66 ug/L	221828	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	80
5			2,3,4-Trimethylpentanoic acid	144	C8H16O2	090435-18-0	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.377	0.6	ug/L	34879	1	6.242	302874	5.0
Methanethiol	1.785	1.3	ug/L	76716	1	6.242	302874	5.0
Ethanethiol	2.467	1.3	ug/L	76005	1	6.242	302874	5.0
Butanoic acid, ...	7.177	3.7	ug/L	221828	1	6.242	302874	5.0