

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011723\
 Data File : VU052719.D
 Acq On : 17 Jan 2023 14:22
 Operator : JC/MD
 Sample : 01138-12 5X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH1X5

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\SFAMUTR011023WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052719.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	97	rVB	75416	89498	15.11%	1.841%
2	1.736	116	123	127	rBV	5000	7465	1.26%	0.154%
3	1.912	171	178	197	rBV	58387	90393	15.26%	1.860%
4	2.472	342	352	367	rBV2	23208	39130	6.60%	0.805%
5	2.565	369	381	395	rVV	135001	221516	37.39%	4.558%
6	2.655	396	409	442	rVV	24468	95928	16.19%	1.974%
7	2.793	443	452	465	rVB2	7523	12626	2.13%	0.260%
8	2.954	491	502	520	rBV	37515	90455	15.27%	1.861%
9	3.044	523	530	541	rVB4	9887	17033	2.87%	0.350%
10	4.639	1010	1026	1045	rBV	56652	193963	32.74%	3.991%
11	5.060	1140	1157	1178	rBV	118701	263334	44.45%	5.418%
12	5.195	1189	1199	1221	rBV2	20847	46713	7.88%	0.961%
13	5.723	1341	1363	1384	rBV3	230192	592454	100.00%	12.190%
14	6.247	1507	1526	1546	rBV	161217	305026	51.49%	6.276%
15	6.395	1565	1572	1584	rVB5	3570	6201	1.05%	0.128%
16	6.687	1648	1663	1682	rBV	145861	282272	47.64%	5.808%
17	7.562	1920	1935	1952	rBV2	65167	114779	19.37%	2.362%
18	7.893	2023	2038	2057	rBV	267602	465010	78.49%	9.568%
19	8.176	2114	2126	2141	rBV	44098	72881	12.30%	1.500%
20	8.468	2205	2217	2234	rBV5	3355	6389	1.08%	0.131%
21	8.632	2256	2268	2300	rBV2	233590	450147	75.98%	9.262%
22	9.414	2499	2511	2531	rBV	226245	375107	63.31%	7.718%
23	10.234	2755	2766	2778	rBV4	4834	7493	1.26%	0.154%
24	10.751	2915	2927	2942	rVB	94911	150934	25.48%	3.106%
25	10.890	2957	2970	2981	rBV3	4235	6379	1.08%	0.131%
26	11.571	3173	3182	3191	rBV2	5119	7639	1.29%	0.157%
27	11.806	3244	3255	3269	rBV	221994	343903	58.05%	7.076%
28	11.877	3270	3277	3289	rVB3	13434	19809	3.34%	0.408%
29	12.189	3356	3374	3395	rBV	243681	394720	66.62%	8.122%
30	12.767	3546	3554	3561	rBV3	12188	18604	3.14%	0.383%
31	12.812	3561	3568	3583	rVB	12794	19995	3.37%	0.411%
32	13.025	3625	3634	3643	rBV3	9950	14931	2.52%	0.307%
33	13.263	3699	3708	3721	rBV5	4377	6775	1.14%	0.139%
34	13.401	3742	3751	3760	rVB3	6183	9210	1.55%	0.190%
35	13.693	3834	3842	3853	rVB3	10945	15019	2.54%	0.309%
36	14.571	4103	4115	4124	rBV	3958	6372	1.08%	0.131%

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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\SFAMUTR011023WMA.M
Title : TRACE VOA SFAM1.0

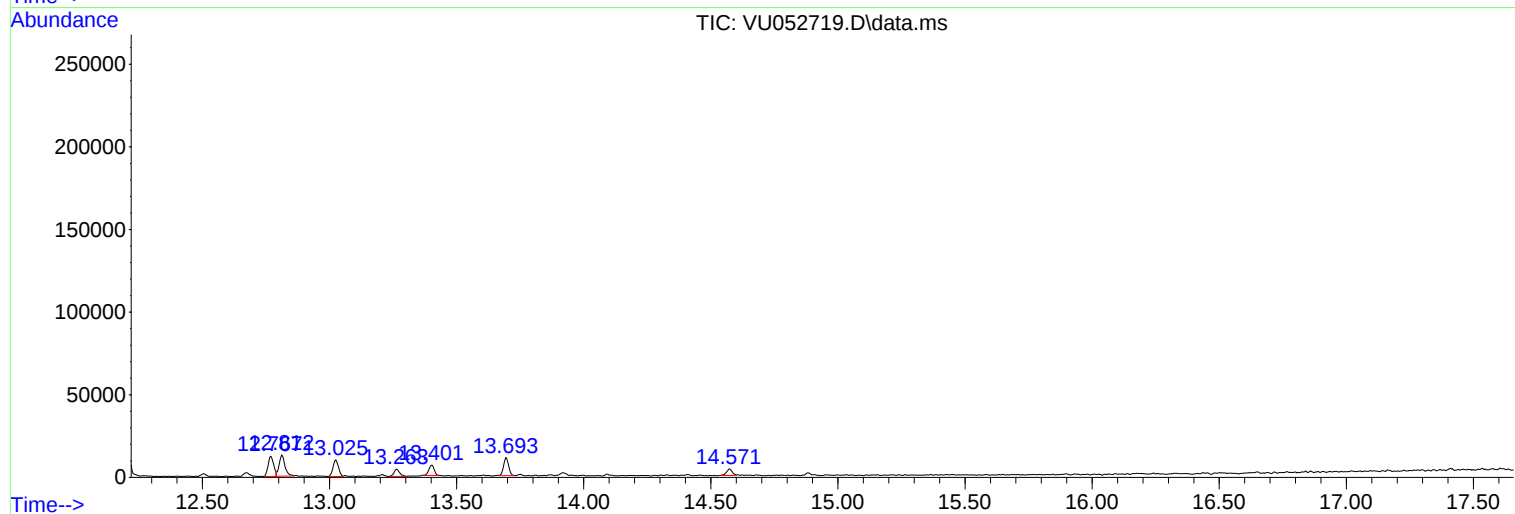
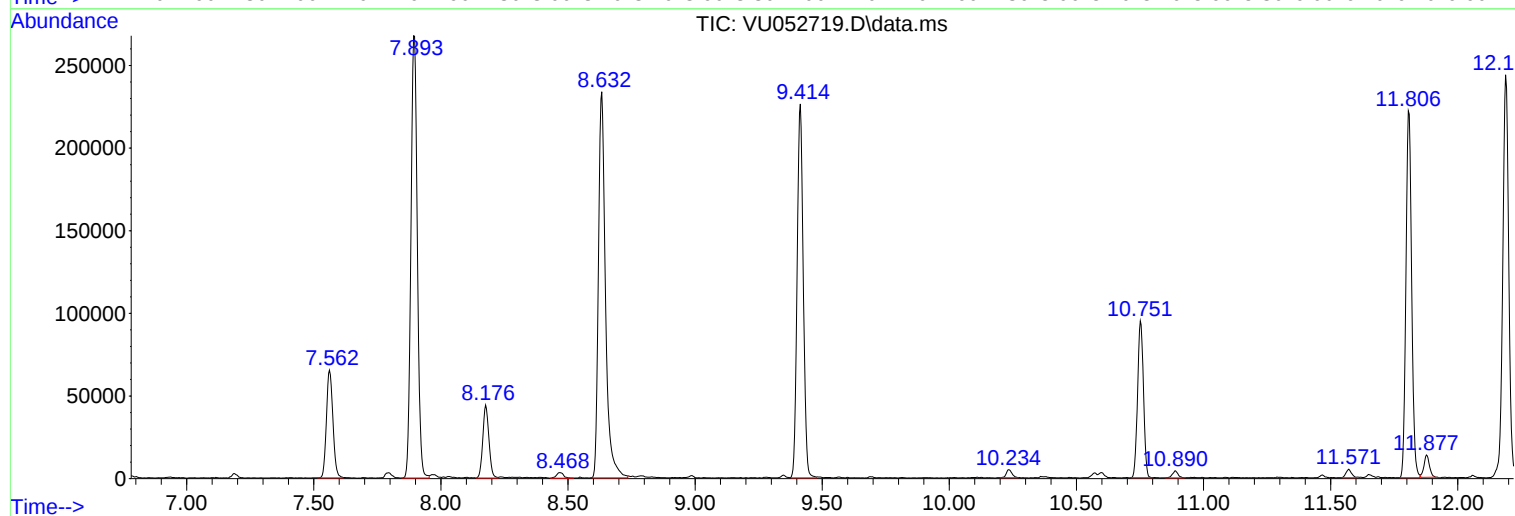
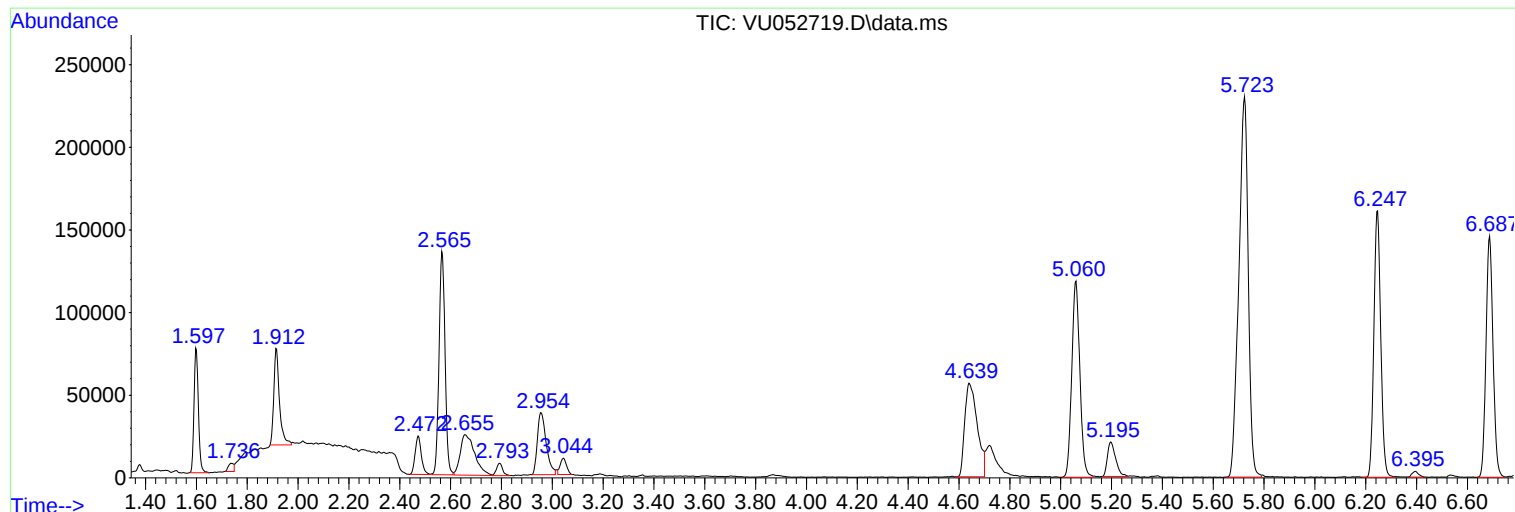
Sum of corrected areas: 4860103

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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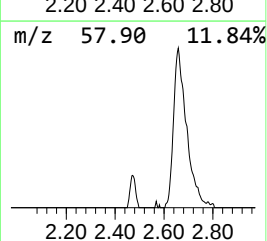
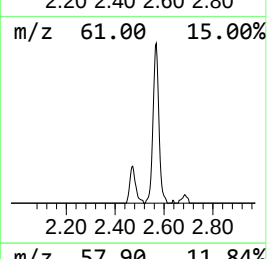
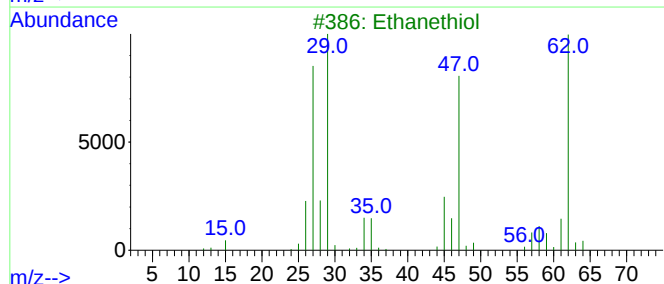
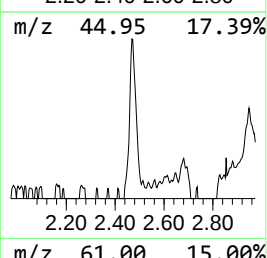
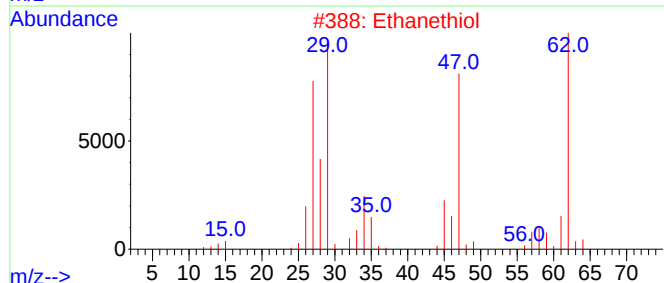
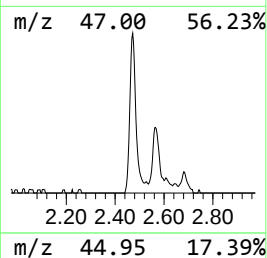
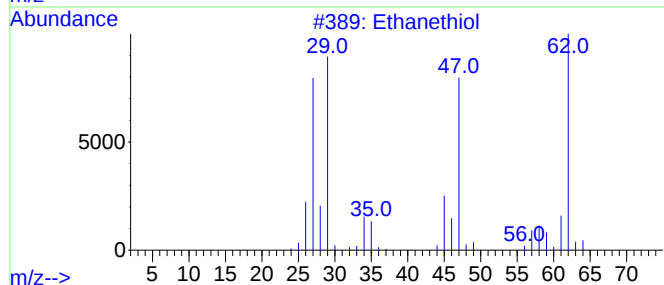
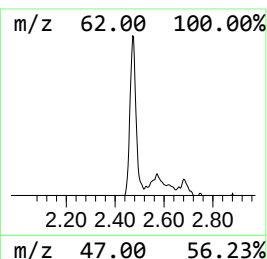
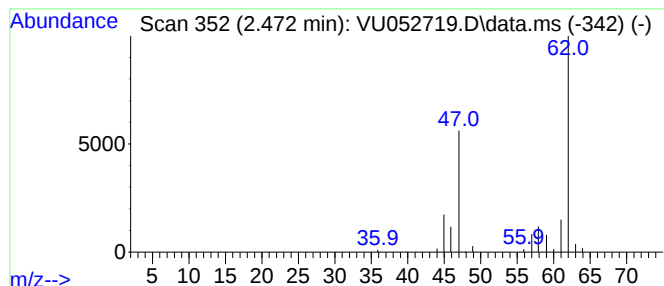
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Ethanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.472	0.64 ug/L	39130	1,4-Difluorobenzene	6.247

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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Instrument :
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ClientSampleId :
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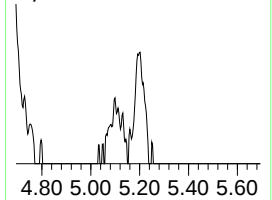
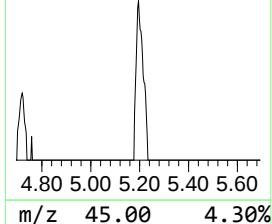
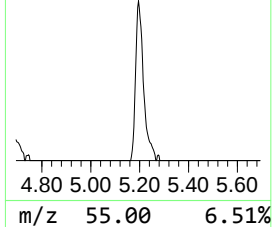
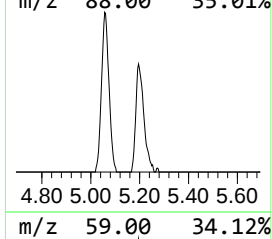
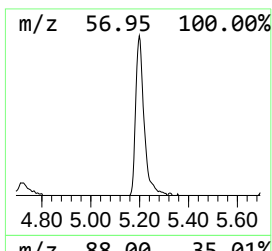
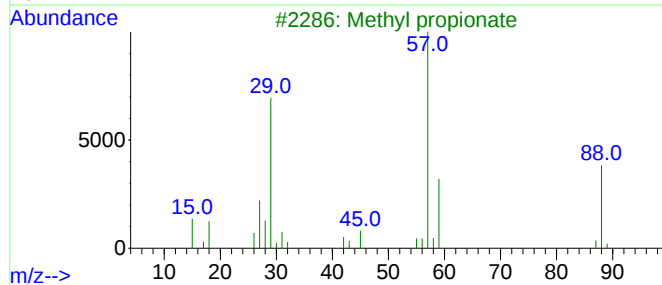
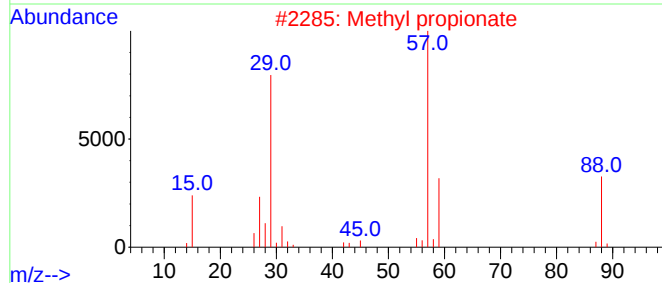
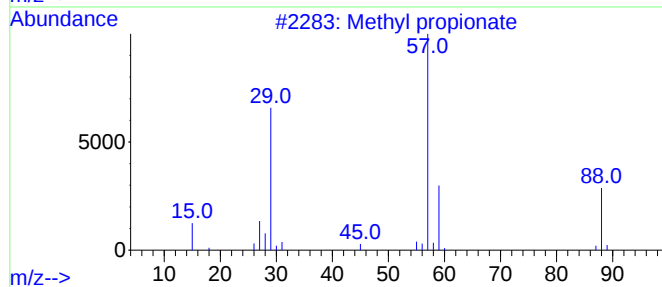
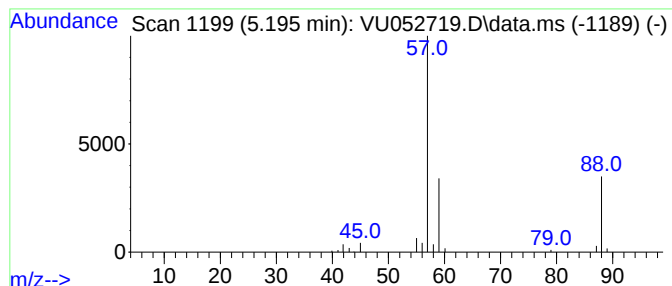
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Methyl propionate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.195	0.77 ug/L	46713	1,4-Difluorobenzene	6.247

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	72



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
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
Ethanethiol	2.472	0.6	ug/L	39130	1	6.247	305026	5.0
Methyl propionate	5.195	0.8	ug/L	46713	1	6.247	305026	5.0