

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051629.D
 Acq On : 31 Oct 2022 23:02
 Operator : JC/MD
 Sample : N5353-16
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBWX1

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\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051629.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	31	40	53	rBV	114585	216007	17.49%	2.788%
2	1.597	74	80	115	rVB2	103122	209855	16.99%	2.708%
3	1.909	170	177	191	rVB	85731	117506	9.52%	1.516%
4	2.080	225	230	241	rVB3	9617	13237	1.07%	0.171%
5	2.565	368	381	393	rBV	110604	179656	14.55%	2.318%
6	3.356	615	627	638	rBV3	7150	14187	1.15%	0.183%
7	3.845	757	779	780	rBV	10162	22823	1.85%	0.295%
8	4.620	1007	1020	1059	rBV	213906	578169	46.82%	7.461%
9	5.060	1141	1157	1188	rBV	174728	407322	32.99%	5.256%
10	5.385	1247	1258	1271	rVB9	7924	16812	1.36%	0.217%
11	5.722	1342	1363	1392	rBV2	303358	845380	68.46%	10.909%
12	6.247	1513	1526	1547	rBV	222739	438768	35.53%	5.662%
13	6.542	1606	1618	1632	rBV2	60535	116063	9.40%	1.498%
14	6.690	1649	1664	1685	rBV	221795	443287	35.90%	5.721%
15	7.565	1923	1936	1955	rBV2	79333	144563	11.71%	1.866%
16	7.896	2024	2039	2057	rBV	277441	488783	39.58%	6.308%
17	8.179	2116	2127	2142	rBV2	50744	89037	7.21%	1.149%
18	8.632	2252	2268	2299	rBV	660403	1234812	100.00%	15.935%
19	9.417	2499	2512	2516	rBV	368517	589941	47.78%	7.613%
20	10.754	2912	2928	2950	rBV	214865	352832	28.57%	4.553%
21	11.812	3245	3257	3281	rVV2	298166	594021	48.11%	7.666%
22	12.060	3324	3334	3347	rBV	39383	74000	5.99%	0.955%
23	12.192	3363	3375	3398	rVB2	303291	562010	45.51%	7.253%

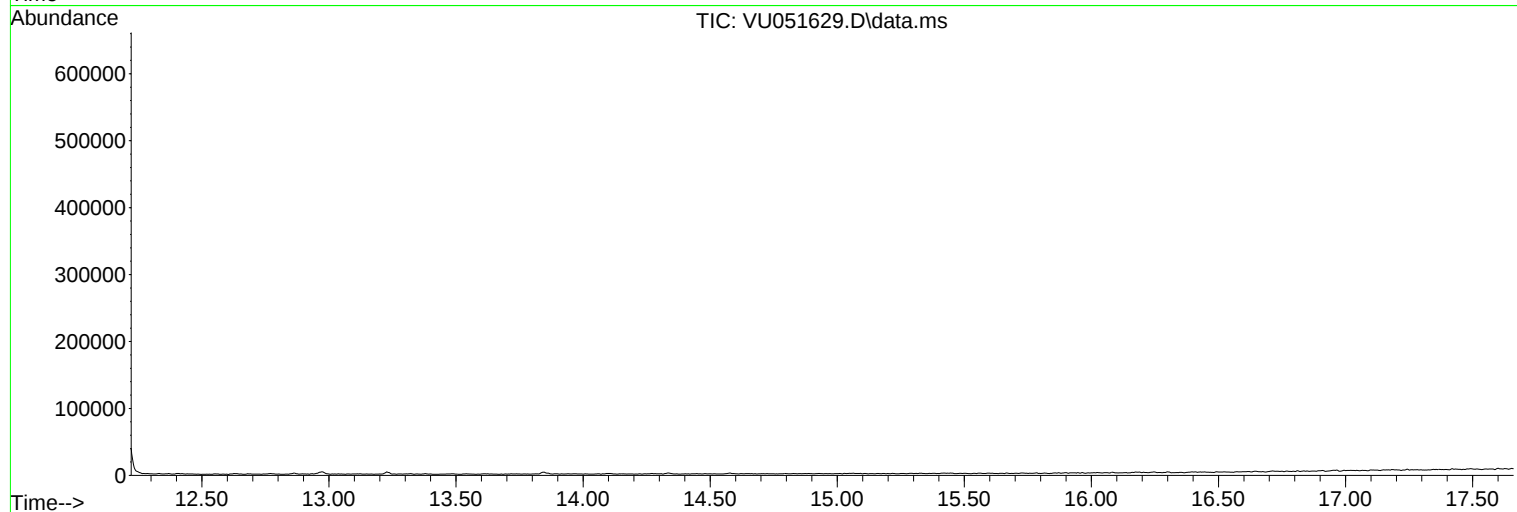
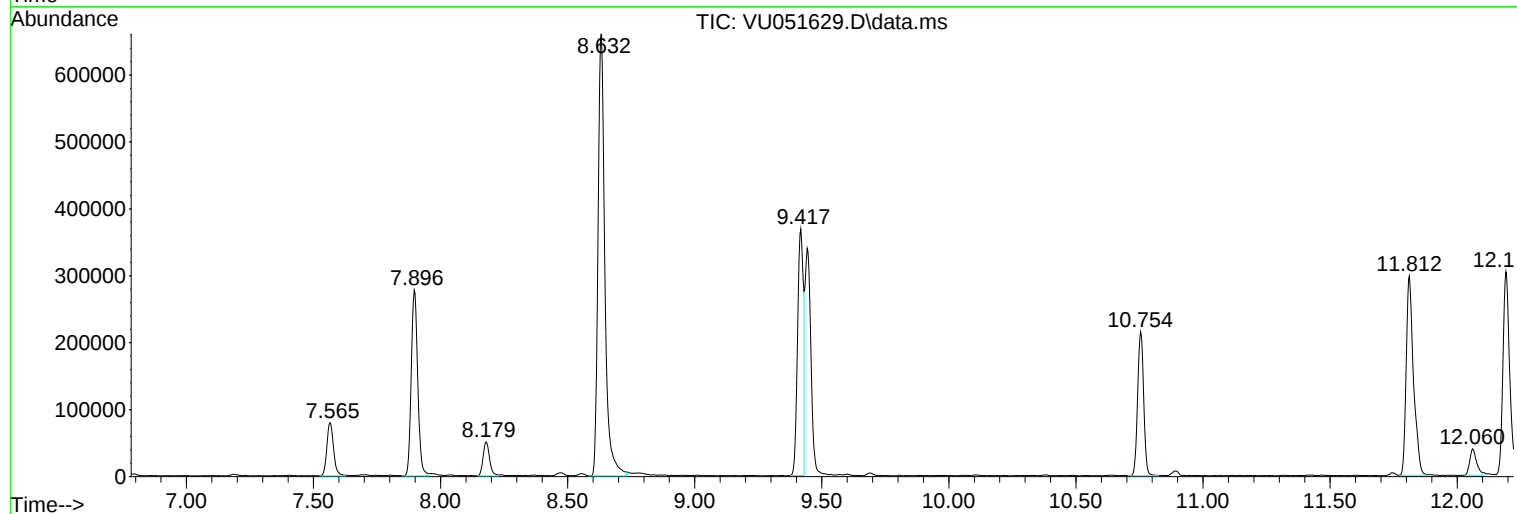
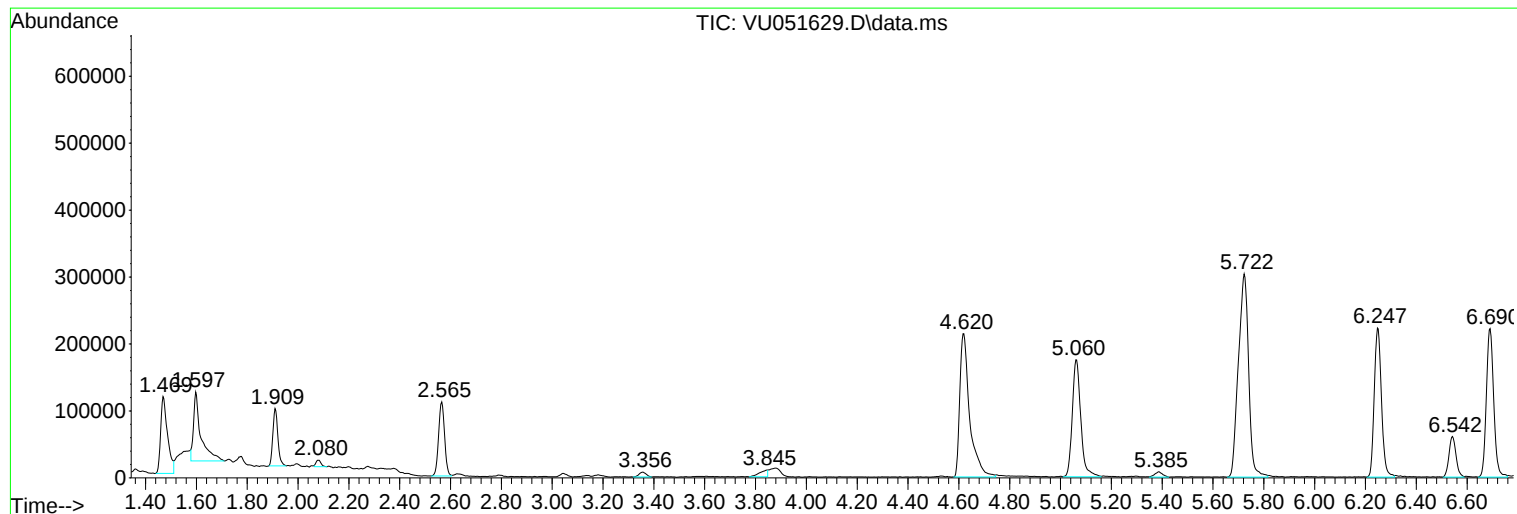
Sum of corrected areas: 7749071

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ALS Vial : 28 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DBWX1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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ClientSampleId :
DBWX1

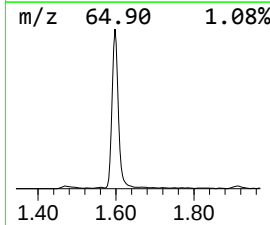
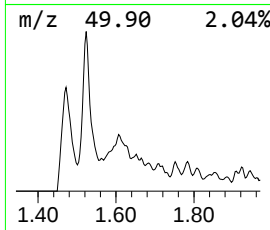
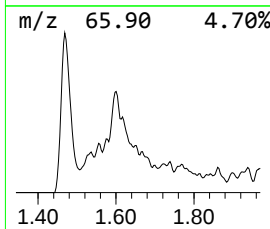
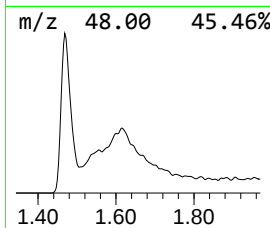
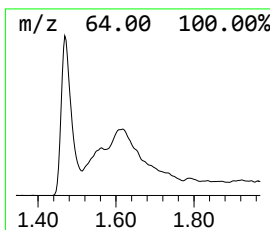
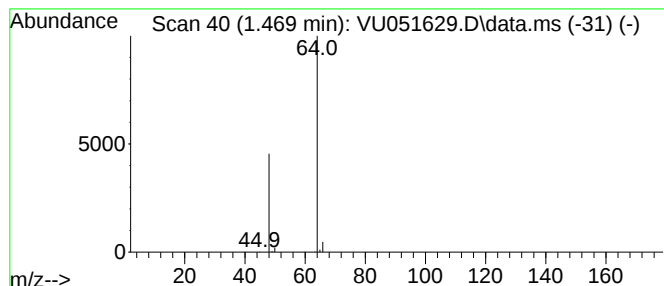
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	2.46 ug/L	216007	1,4-Difluorobenzene	6.250

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			Sulfur dioxide	64	O2S	007446-09-5	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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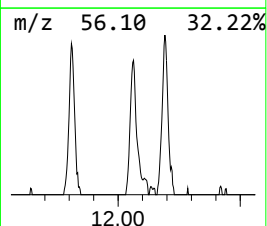
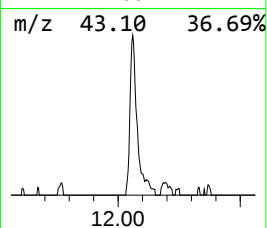
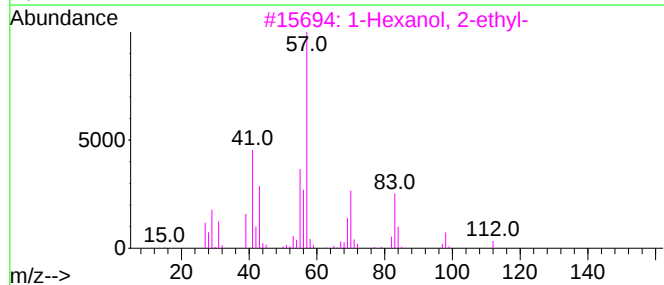
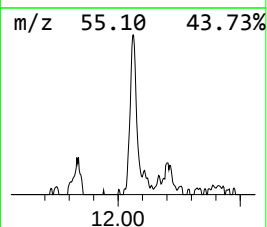
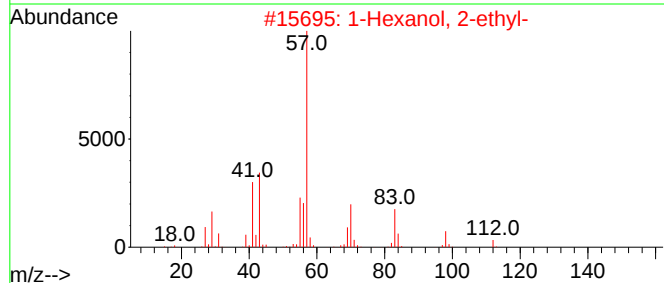
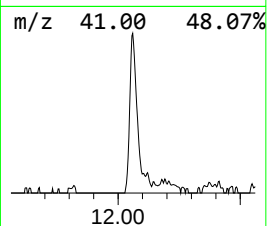
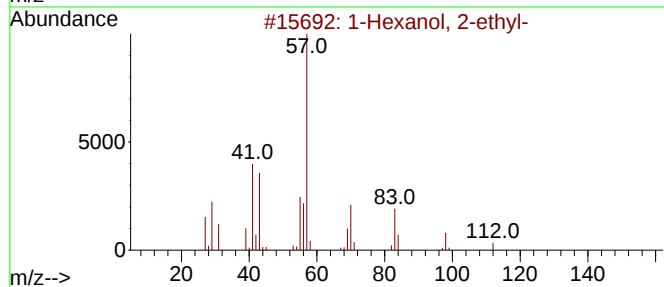
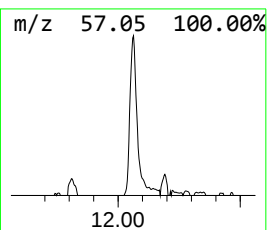
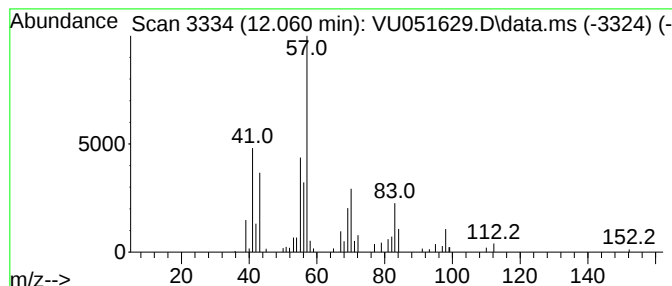
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	0.62 ug/L	74000	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	64



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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	1.469	2.5	ug/L	216007	1	6.250	438768	5.0
1-Hexanol, 2-et...	12.060	0.6	ug/L	74000	3	11.809	594021	5.0