

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
 Data File : VU051736.D
 Acq On : 03 Nov 2022 16:14
 Operator : JC/MD
 Sample : N5407-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4Y4

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: VU051736.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.366	3	8	13	rBV	11692	15656	2.17%	0.223%
2	1.491	42	47	50	rBV3	14164	16782	2.33%	0.239%
3	1.536	51	61	82	rBV	188282	720923	100.00%	10.263%
4	1.626	85	89	98	rVB	79781	106298	14.74%	1.513%
5	2.597	382	391	405	rVB	136291	221304	30.70%	3.151%
6	2.825	456	462	475	rVB	20399	33277	4.62%	0.474%
7	4.735	1040	1056	1091	rVB2	65155	268214	37.20%	3.818%
8	5.089	1154	1166	1183	rVB	141985	293167	40.67%	4.174%
9	5.761	1352	1375	1403	rBV3	238797	650637	90.25%	9.263%
10	5.992	1441	1447	1470	rBV3	10185	21031	2.92%	0.299%
11	6.317	1533	1548	1566	rBV	228922	423681	58.77%	6.032%
12	6.751	1667	1683	1710	rBV	164429	320810	44.50%	4.567%
13	7.603	1936	1948	1967	rBV2	71076	126511	17.55%	1.801%
14	7.928	2037	2049	2063	rBV	258811	446657	61.96%	6.359%
15	8.002	2064	2072	2083	rVB	15567	28909	4.01%	0.412%
16	8.208	2125	2136	2150	rBV	43171	74152	10.29%	1.056%
17	8.494	2213	2225	2238	rBV2	9246	17678	2.45%	0.252%
18	8.574	2241	2250	2258	rBV8	4396	7732	1.07%	0.110%
19	8.664	2261	2278	2311	rBV	340646	699474	97.02%	9.958%
20	9.433	2503	2517	2535	rBV	326485	551757	76.53%	7.855%
21	9.706	2593	2602	2611	rBV5	5800	9095	1.26%	0.129%
22	10.024	2659	2701	2717	rBV5	33346	211126	29.29%	3.006%
23	10.761	2916	2930	2944	rVB	138614	226962	31.48%	3.231%
24	10.896	2960	2972	2987	rVB3	18169	32625	4.53%	0.464%
25	11.812	3246	3257	3278	rVB	337247	552592	76.65%	7.867%
26	12.066	3322	3336	3361	rBV3	49031	134170	18.61%	1.910%
27	12.195	3364	3376	3392	rVB	282421	468930	65.05%	6.676%
28	12.539	3472	3483	3512	rBV4	66807	160453	22.26%	2.284%
29	12.770	3546	3555	3563	rBV2	6057	9792	1.36%	0.139%
30	12.886	3584	3591	3603	rVB9	6356	10403	1.44%	0.148%
31	13.208	3682	3691	3701	rBV4	15121	23748	3.29%	0.338%
32	14.034	3942	3948	3956	rVB8	7758	11277	1.56%	0.161%
33	14.420	4059	4068	4077	rVB	19399	30026	4.16%	0.427%
34	14.574	4107	4116	4124	rVB2	4231	7390	1.03%	0.105%
35	15.481	4389	4398	4407	rBV4	7907	12669	1.76%	0.180%
36	16.185	4607	4617	4624	rBV4	6792	11543	1.60%	0.164%

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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\SFAMUTR102822WMA.M
Title : TRACE VOA SFAM1.0

37	16.230	4624	4631	4642	rVV3	14280	20678	2.87%	0.294%
38	16.516	4708	4720	4729	rVB10	8328	16837	2.34%	0.240%
39	16.764	4789	4797	4810	rVB5	18945	29385	4.08%	0.418%

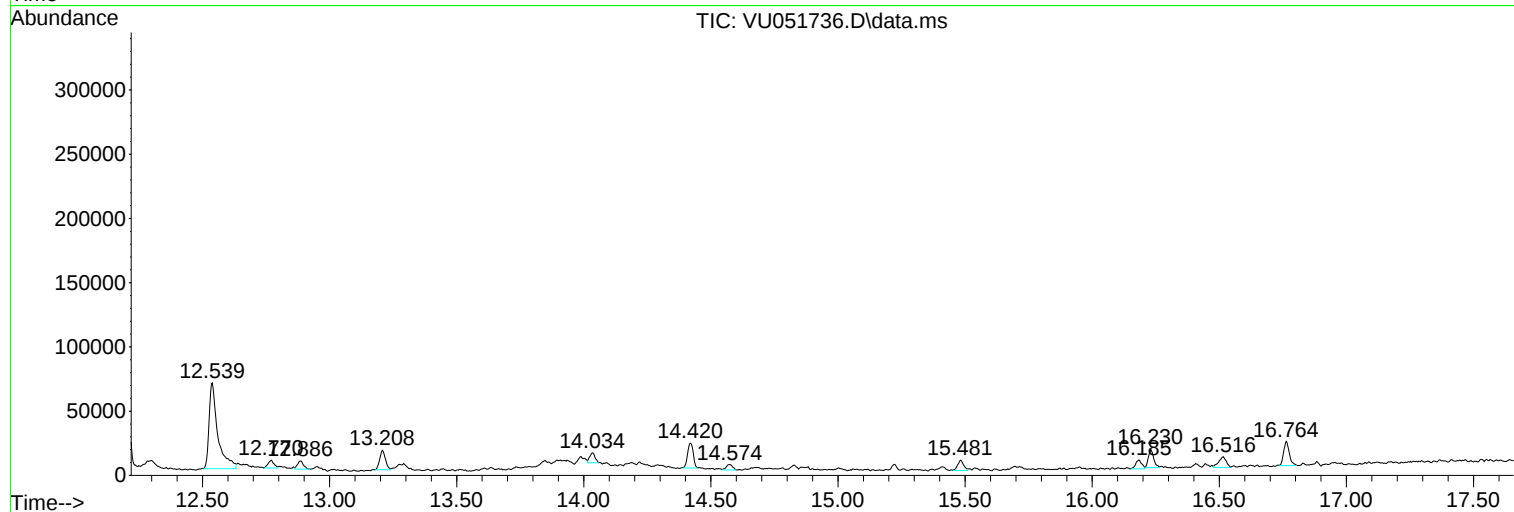
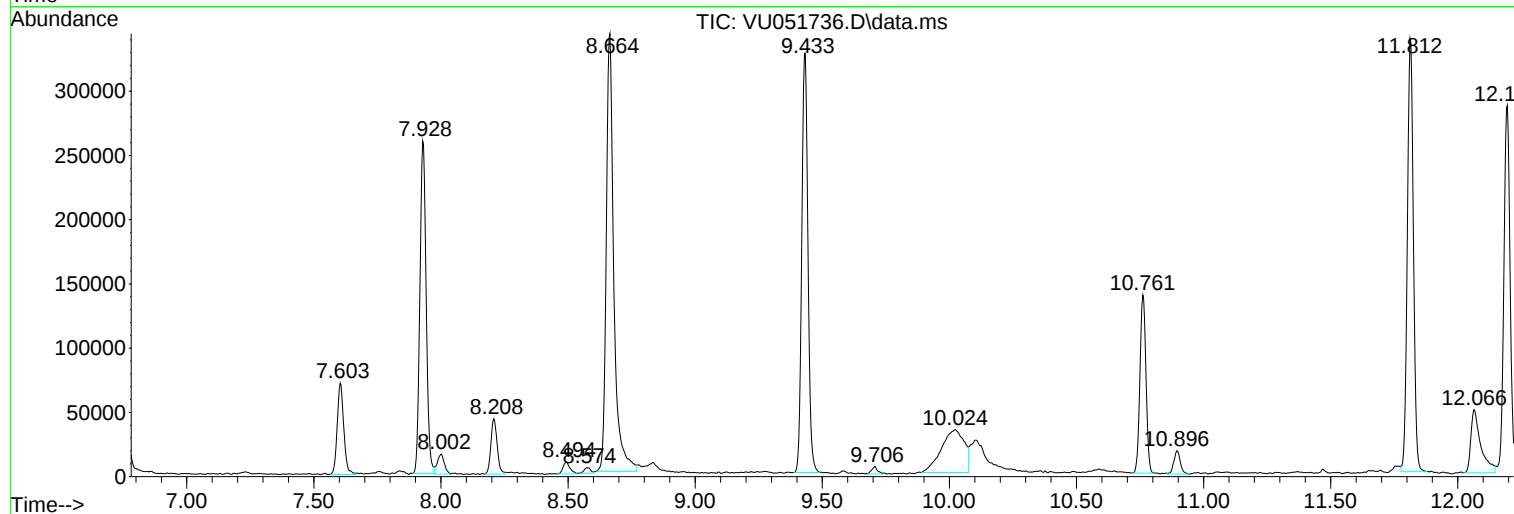
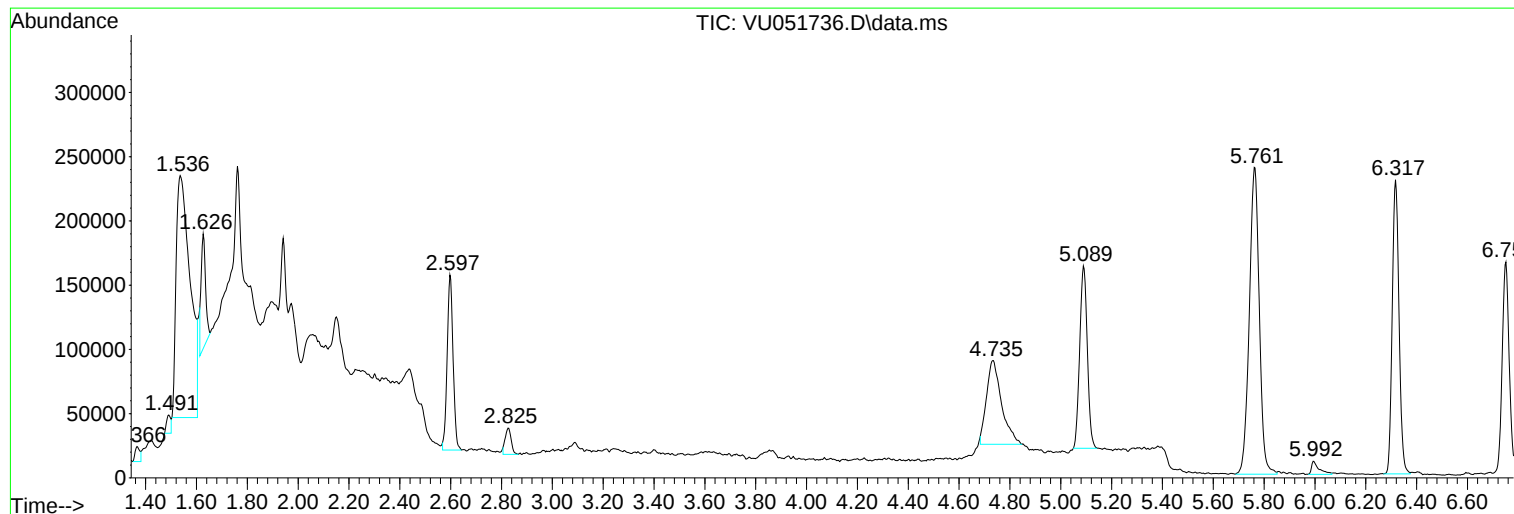
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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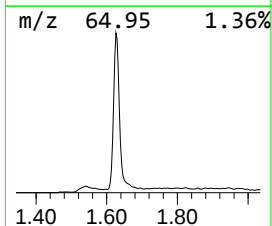
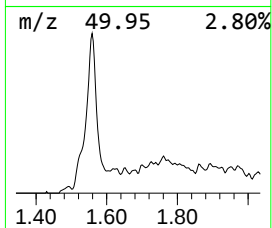
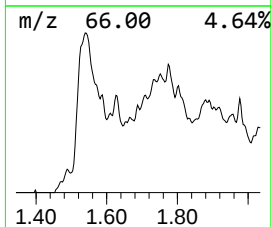
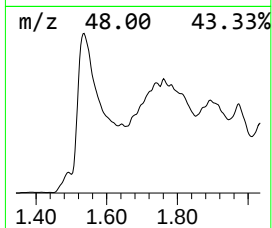
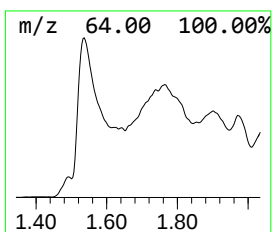
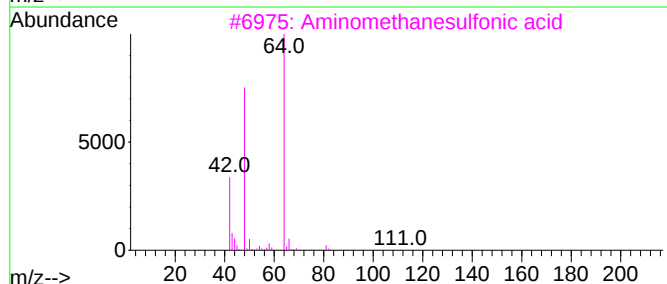
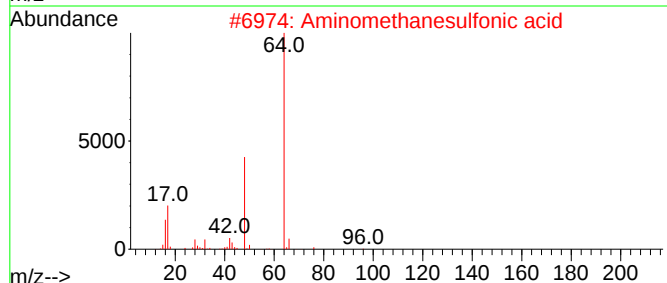
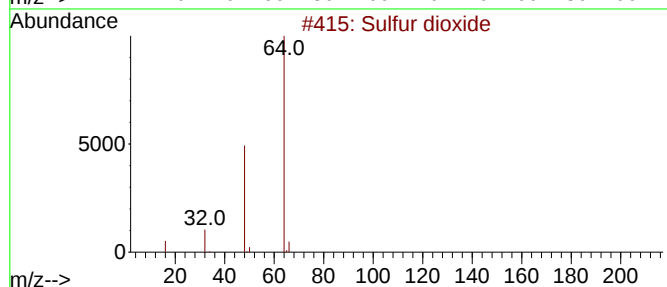
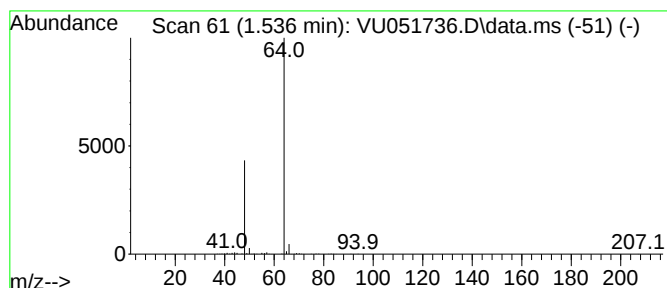
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.536	8.51 ug/L	720923	1,4-Difluorobenzene	6.317

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	25
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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ALS Vial : 15 Sample Multiplier: 1

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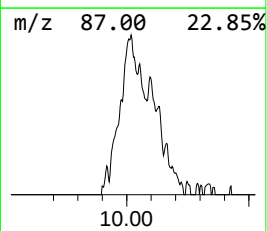
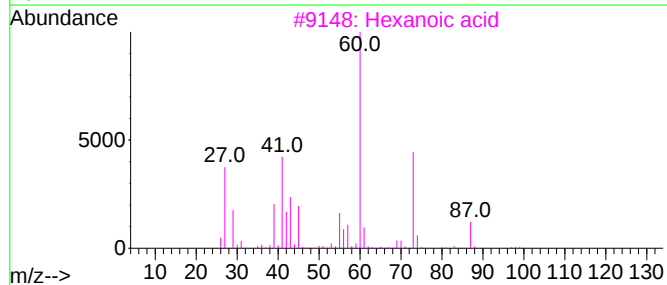
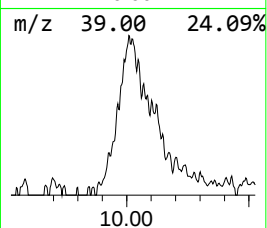
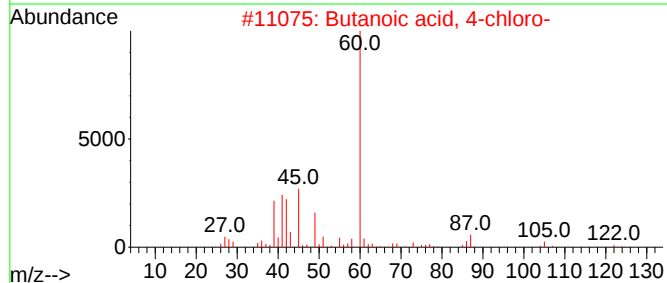
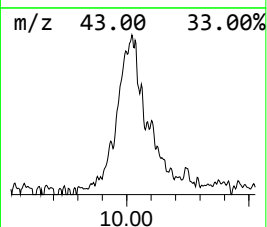
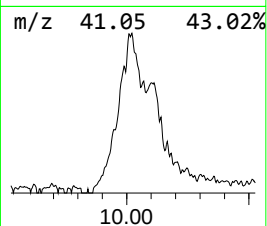
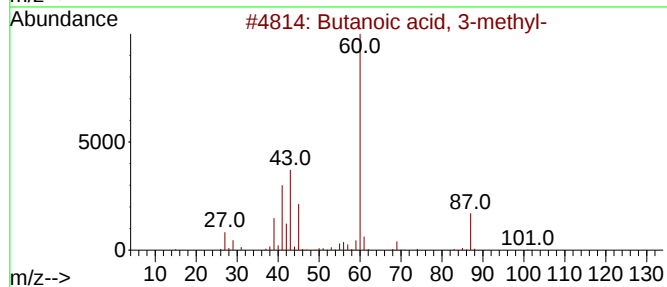
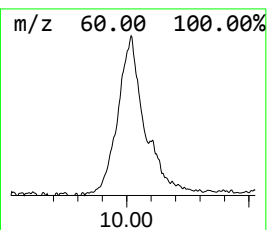
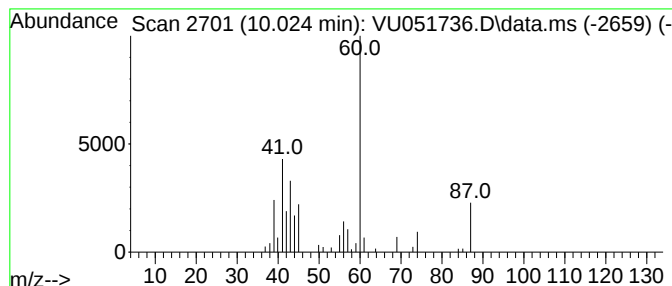
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Butanoic acid, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.025	1.91 ug/L	211126	Chlorobenzene-d5	9.433

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
2			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	59
3			Hexanoic acid	116	C6H12O2	000142-62-1	59
4			Hexanoic acid	116	C6H12O2	000142-62-1	56
5			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53



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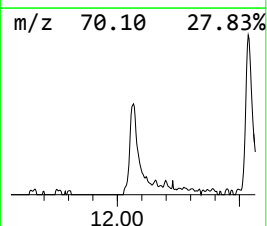
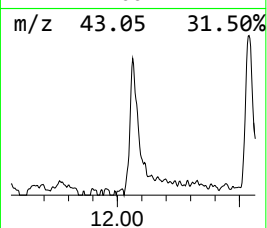
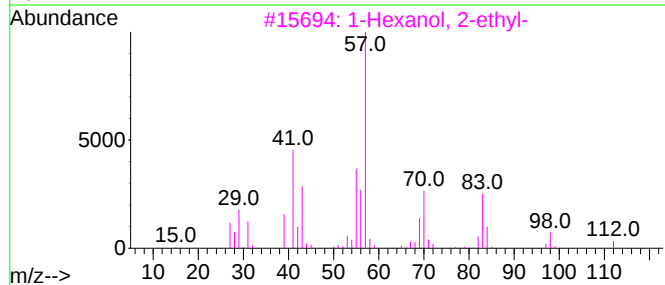
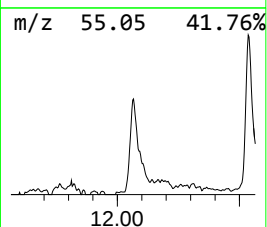
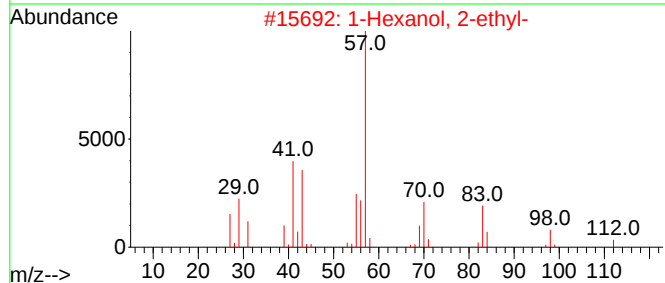
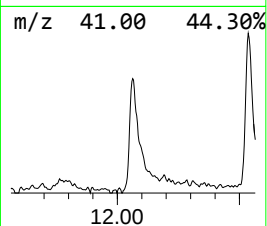
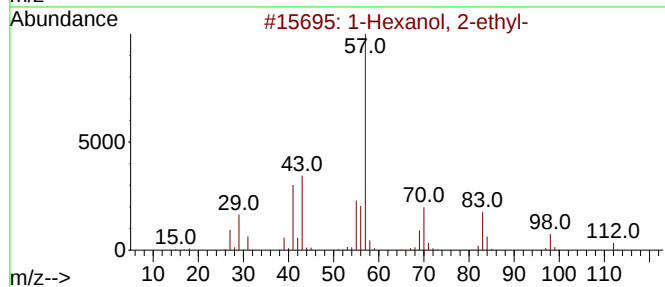
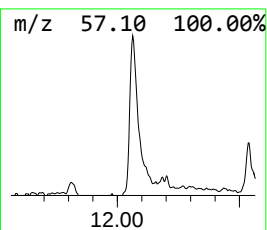
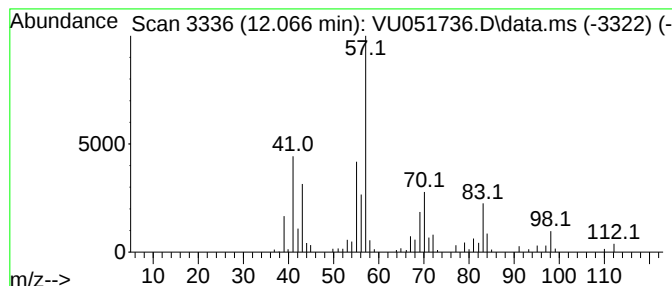
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.066	1.21 ug/L	134170	1,4-Dichlorobenzene-d4	11.815

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			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



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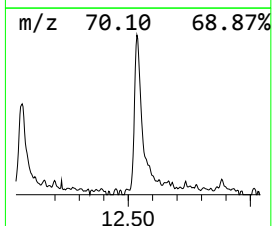
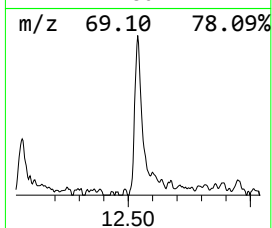
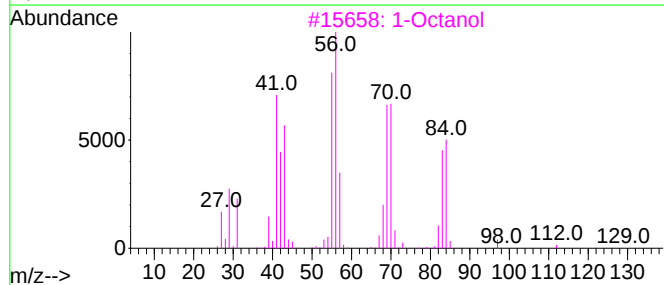
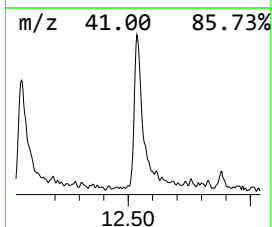
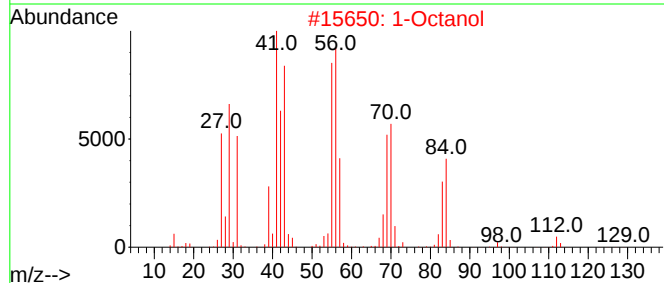
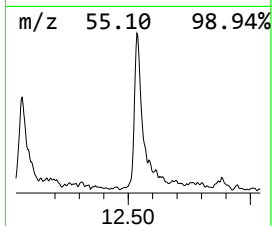
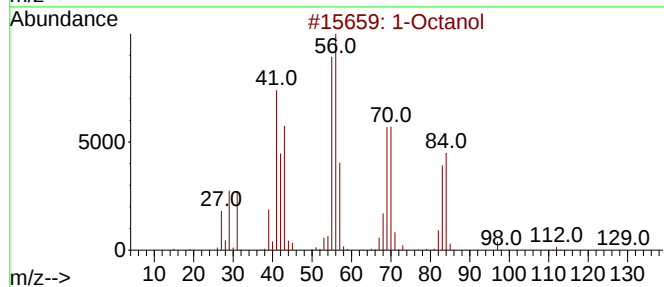
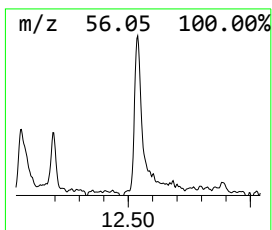
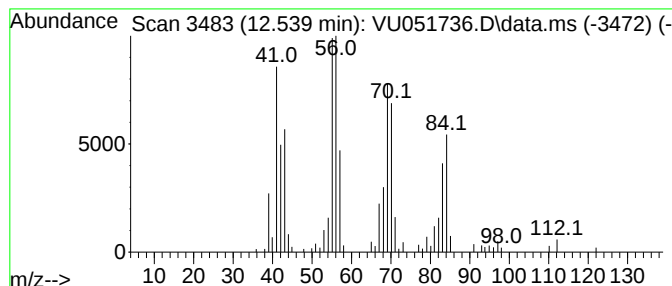
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	1.45 ug/L	160453	1,4-Dichlorobenzene-d4	11.815

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	86
2			1-Octanol	130	C8H18O	000111-87-5	86
3			1-Octanol	130	C8H18O	000111-87-5	78
4			1-Nonanol	144	C9H20O	000143-08-8	72
5			Cycloheptane	98	C7H14	000291-64-5	58



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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
Sulfur dioxide	1.536	8.5	ug/L	720923	1	6.317	423681	5.0
Butanoic acid, ...	10.025	1.9	ug/L	211126	2	9.433	551757	5.0
1-Hexanol, 2-et...	12.066	1.2	ug/L	134170	3	11.815	552592	5.0
1-Octanol	12.539	1.5	ug/L	160453	3	11.815	552592	5.0