

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090523\
 Data File : VU055091.D
 Acq On : 05 Sep 2023 14:00
 Operator : MD/SY
 Sample : 04267-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH4F1

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\SFAMUTR090123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU055091.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	15	20	33	rBV3	6527	10337	1.70%	0.162%
2	1.480	52	59	67	rBV	62483	62564	10.31%	0.981%
3	1.595	87	95	105	rVB	50524	57698	9.51%	0.905%
4	1.907	184	192	205	rBV	63737	81930	13.51%	1.285%
5	2.563	384	396	407	rBV2	117750	191135	31.51%	2.998%
6	2.628	407	416	440	rVB	66392	120255	19.83%	1.886%
7	2.785	453	465	473	rBV9	2780	6163	1.02%	0.097%
8	2.952	505	517	533	rBV	19364	38019	6.27%	0.596%
9	3.042	534	545	559	rVB	14629	26471	4.36%	0.415%
10	4.627	1027	1038	1058	rBV	87385	226149	37.28%	3.547%
11	4.820	1092	1098	1109	rVB2	5725	9673	1.59%	0.152%
12	5.058	1157	1172	1197	rBV	138279	317906	52.41%	4.986%
13	5.724	1359	1379	1400	rBV3	231541	606582	100.00%	9.513%
14	6.248	1529	1542	1562	rBV	206524	399302	65.83%	6.262%
15	6.534	1622	1631	1644	rBV9	7471	16549	2.73%	0.260%
16	6.688	1666	1679	1702	rBV	150643	301139	49.65%	4.723%
17	6.975	1759	1768	1785	rVB6	3577	7867	1.30%	0.123%
18	7.566	1941	1952	1969	rBV2	55805	102558	16.91%	1.608%
19	7.795	2013	2023	2043	rBV3	15405	29083	4.79%	0.456%
20	7.897	2043	2055	2069	rVV	278198	493703	81.39%	7.743%
21	7.971	2069	2078	2097	rVB	35098	66314	10.93%	1.040%
22	8.180	2133	2143	2160	rBV2	33793	60781	10.02%	0.953%
23	8.634	2273	2284	2319	rBV2	268015	600717	99.03%	9.421%
24	8.788	2322	2332	2339	rVV2	55830	95350	15.72%	1.495%
25	8.833	2339	2346	2369	rVB	119028	205790	33.93%	3.227%
26	9.415	2516	2527	2550	rBV	308108	533665	87.98%	8.369%
27	9.573	2565	2576	2586	rBV3	7233	11498	1.90%	0.180%
28	9.695	2604	2614	2630	rBV2	16533	30264	4.99%	0.475%
29	10.116	2729	2745	2766	rBV5	29021	70875	11.68%	1.112%
30	10.241	2772	2784	2794	rBV4	8902	16152	2.66%	0.253%
31	10.344	2803	2816	2830	rBV9	9380	20682	3.41%	0.324%
32	10.756	2932	2944	2962	rBV	113407	184808	30.47%	2.898%
33	10.891	2975	2986	2996	rBV4	5529	8412	1.39%	0.132%
34	11.479	3158	3169	3183	rBV3	9376	17317	2.85%	0.272%
35	11.685	3225	3233	3244	rBV4	10762	17621	2.90%	0.276%
36	11.810	3260	3272	3293	rBV	360203	583900	96.26%	9.157%

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Title : TRACE VOA SFAM1.0

37	11.910	3293	3303	3311	rVB9	5752	9090	1.50%	0.143%
38	12.058	3337	3349	3374	rBV	91144	196434	32.38%	3.081%
39	12.193	3379	3391	3408	rVB	290566	482743	79.58%	7.571%
40	12.778	3563	3573	3584	rVB6	8033	13201	2.18%	0.207%
41	12.888	3599	3607	3617	rBV4	19484	29332	4.84%	0.460%
42	13.212	3696	3708	3716	rBV7	5659	9771	1.61%	0.153%
43	14.097	3971	3983	3989	rBV4	4607	6622	1.09%	0.104%

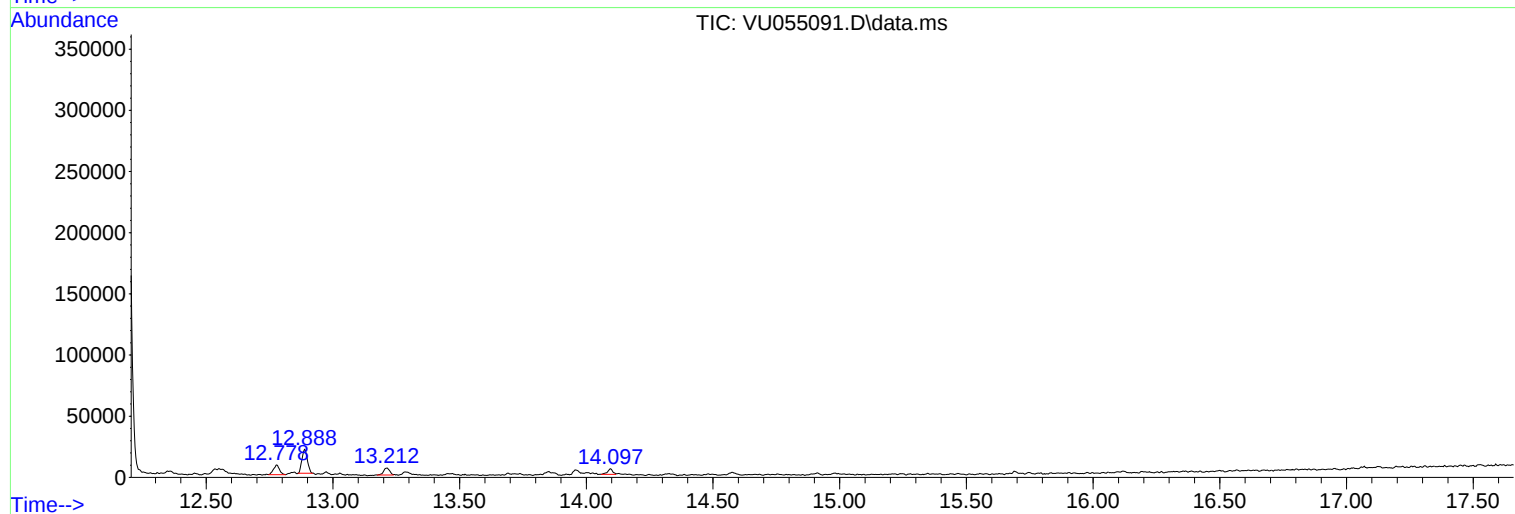
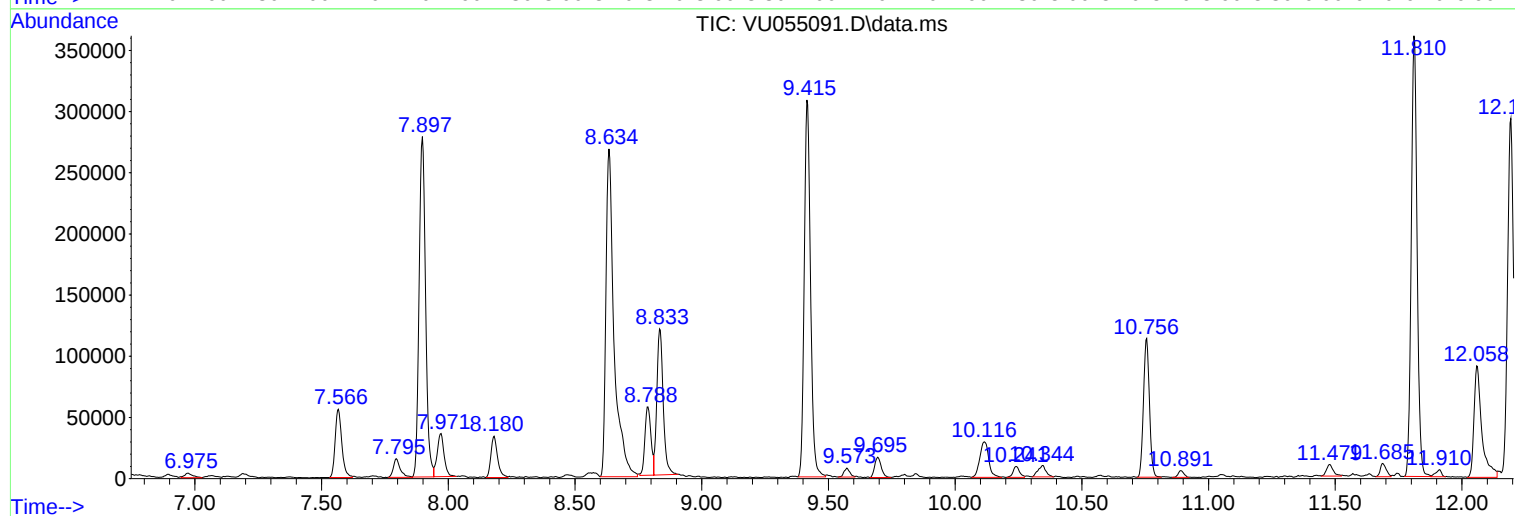
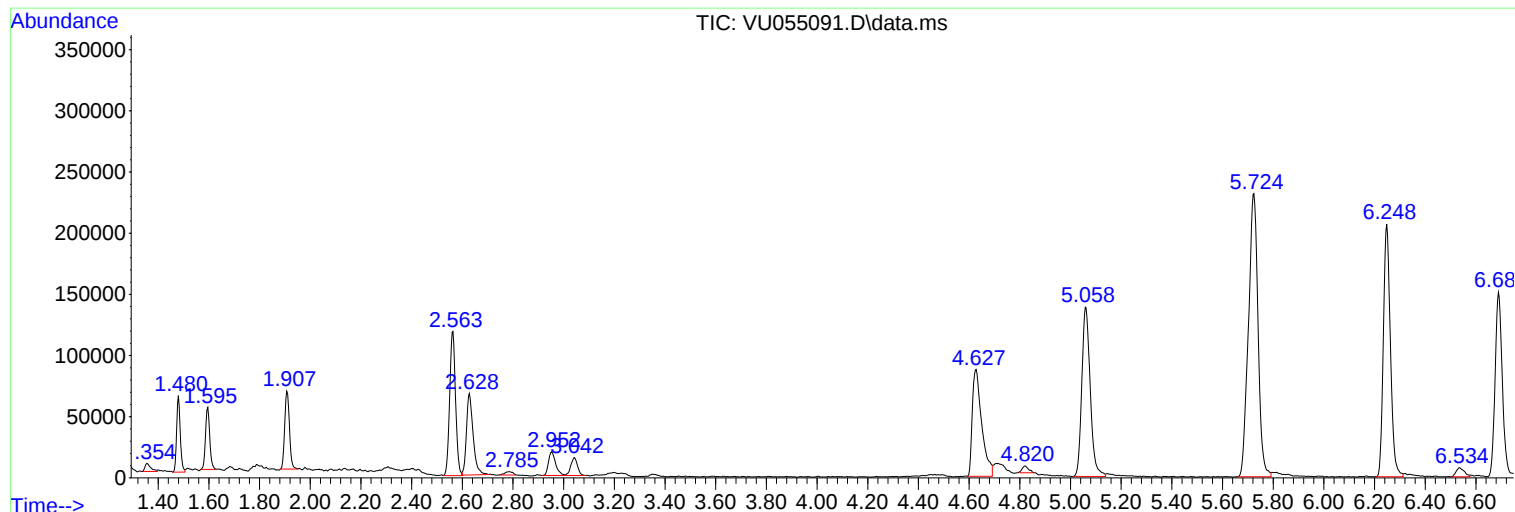
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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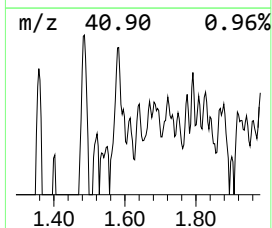
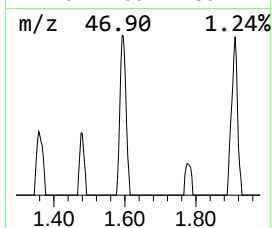
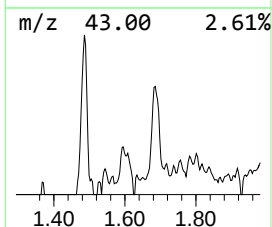
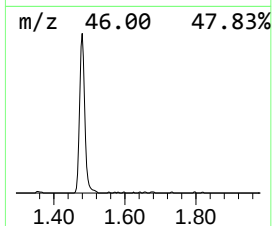
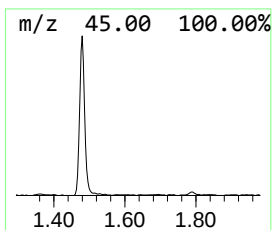
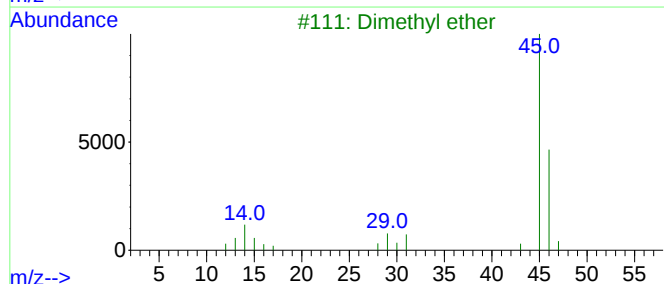
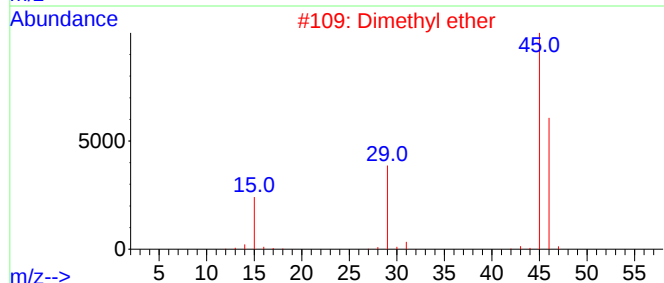
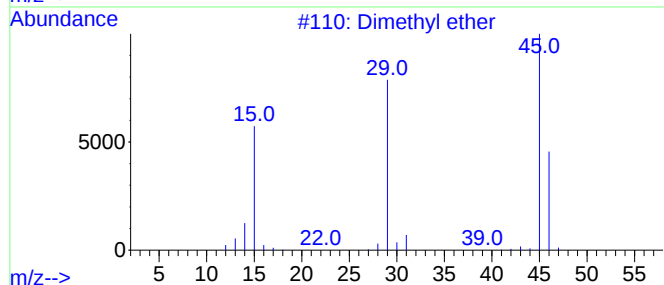
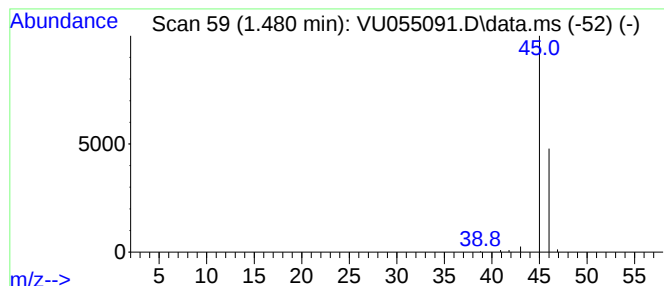
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Dimethyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.480	0.78 ug/L	62564	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	74
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Dimethyl ether	46	C2H6O	000115-10-6	7
4			Ethanol	46	C2H6O	000064-17-5	7
5			Ethanol	46	C2H6O	000064-17-5	7



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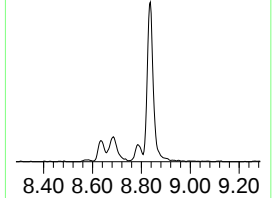
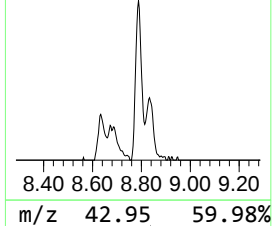
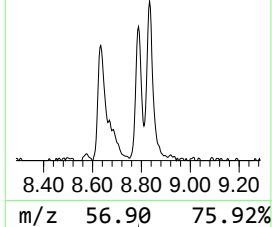
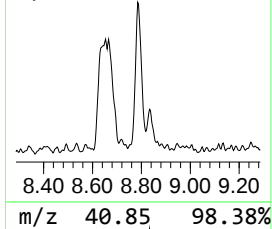
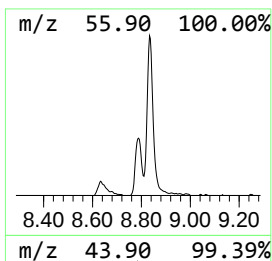
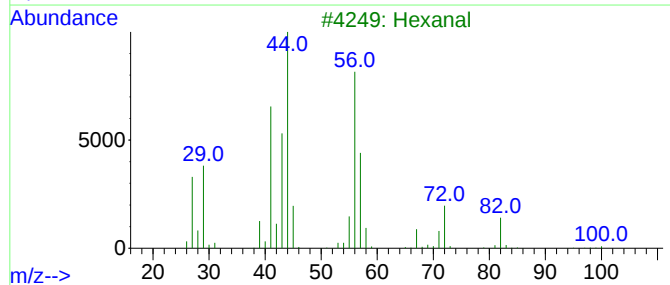
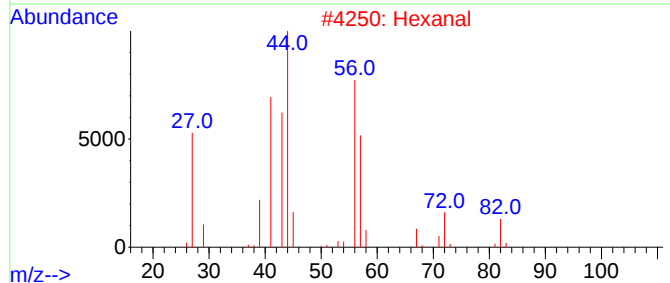
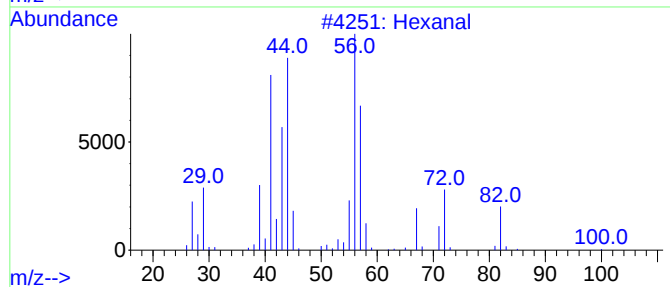
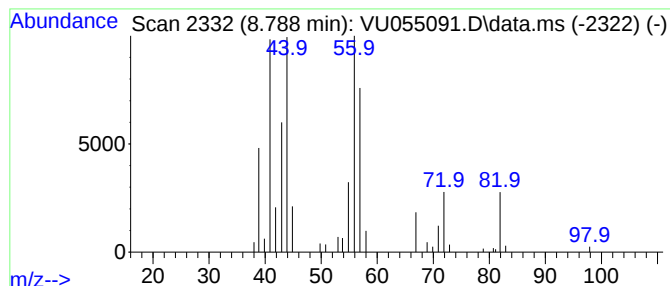
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.788	0.89 ug/L	95350	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	64
2	Hexanal			100	C6H12O	000066-25-1	59
3	Hexanal			100	C6H12O	000066-25-1	59
4	Hexanal			100	C6H12O	000066-25-1	53
5	Hexanal			100	C6H12O	000066-25-1	53



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
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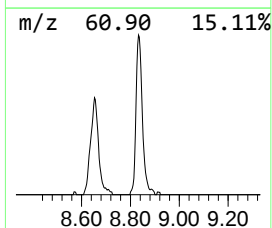
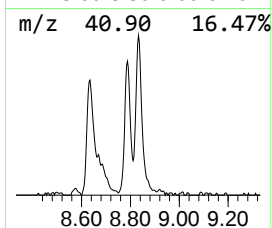
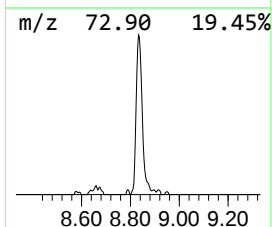
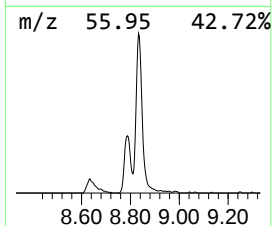
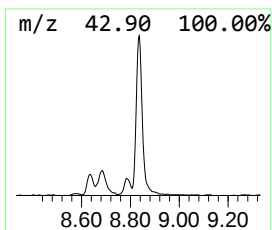
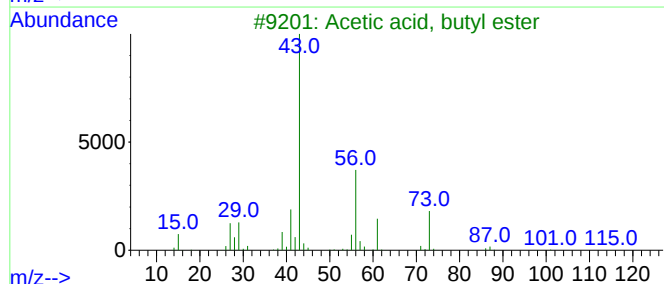
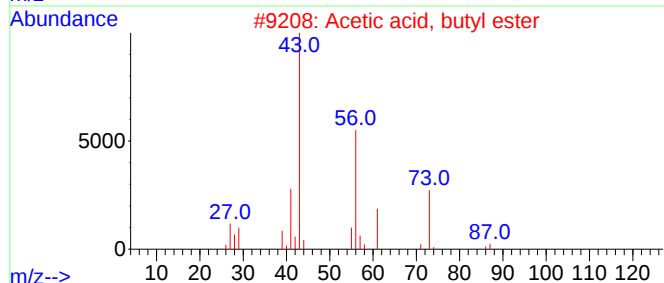
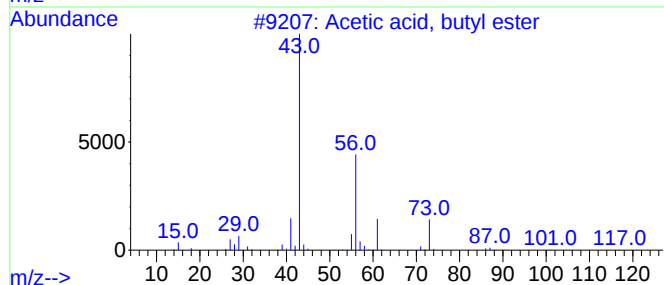
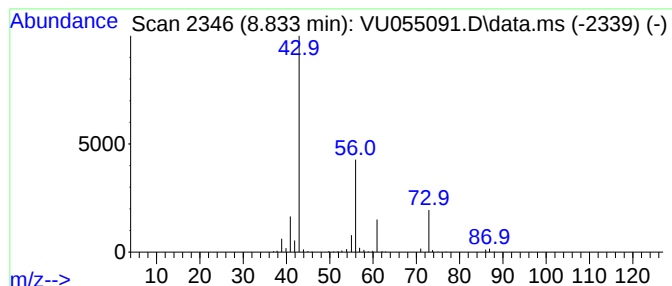
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Acetic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.833	1.93 ug/L	205790	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	56
5			2-Pentanone	86	C5H10O	000107-87-9	9



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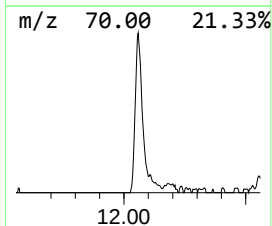
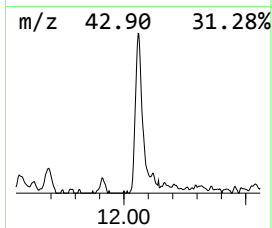
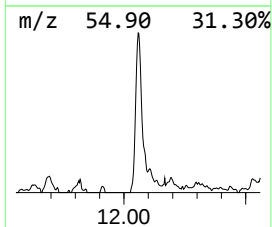
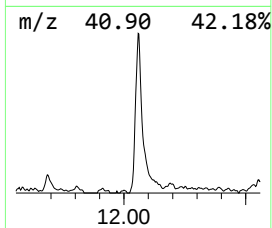
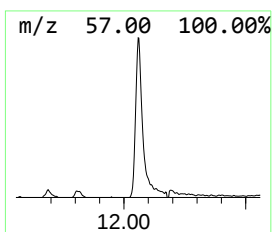
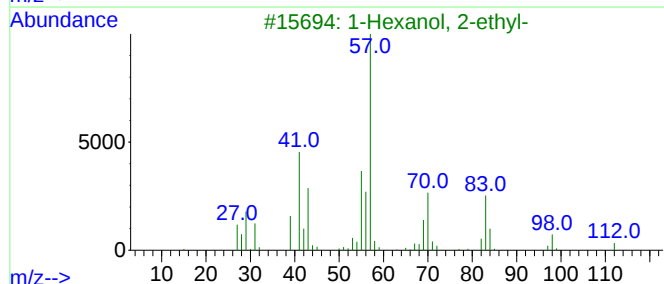
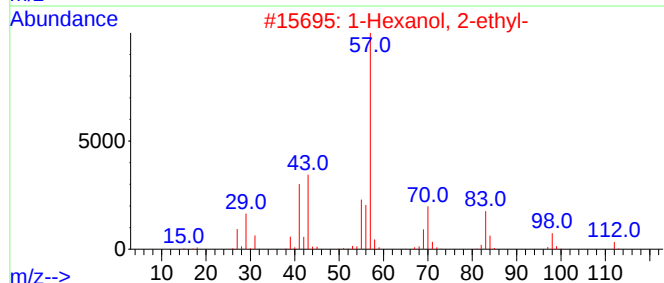
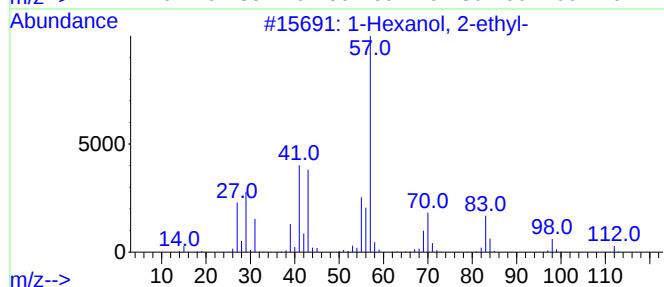
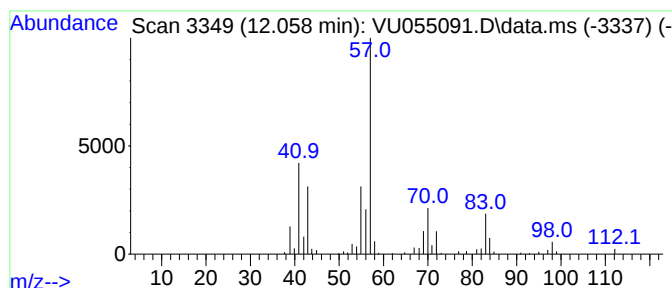
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.058	1.68 ug/L	196434	1,4-Dichlorobenzene-d4	11.810

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	72
5			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56



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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
Dimethyl ether	1.480	0.8	ug/L	62564	1	6.248	399302	5.0
Hexanal	8.788	0.9	ug/L	95350	2	9.415	533665	5.0
Acetic acid, bu...	8.833	1.9	ug/L	205790	2	9.415	533665	5.0
1-Hexanol, 2-et...	12.058	1.7	ug/L	196434	3	11.810	583900	5.0