

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090623\
 Data File : VU055135.D
 Acq On : 06 Sep 2023 13:09
 Operator : MD/SY
 Sample : 04267-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 5 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: VU055135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.355	15	20	25	rBV3	5456	6479	1.06%	0.105%
2	1.480	52	59	67	rBV	57039	56999	9.35%	0.924%
3	1.596	87	95	106	rVB	49486	56992	9.35%	0.924%
4	1.908	184	192	203	rBV	60603	77454	12.70%	1.255%
5	2.560	383	395	408	rBV	113826	184090	30.19%	2.983%
6	2.631	408	417	442	rVB	58007	119203	19.55%	1.932%
7	2.953	506	517	532	rBV	19363	37803	6.20%	0.613%
8	3.043	535	545	557	rVB4	12556	22893	3.75%	0.371%
9	3.586	701	714	723	rBV3	4181	9673	1.59%	0.157%
10	4.631	1028	1039	1059	rBV	81305	216192	35.45%	3.504%
11	5.062	1157	1173	1196	rBV2	129520	302513	49.61%	4.903%
12	5.724	1360	1379	1408	rBV2	222233	587985	96.42%	9.529%
13	6.248	1529	1542	1561	rBV	226684	433634	71.11%	7.028%
14	6.538	1622	1632	1647	rBV9	7069	15398	2.53%	0.250%
15	6.689	1666	1679	1698	rBV	142896	288920	47.38%	4.682%
16	7.566	1938	1952	1968	rBV	53209	96589	15.84%	1.565%
17	7.795	2013	2023	2037	rBV2	13212	25546	4.19%	0.414%
18	7.898	2043	2055	2070	rBV	265925	468398	76.81%	7.591%
19	7.972	2070	2078	2092	rVB2	29708	54567	8.95%	0.884%
20	8.181	2129	2143	2158	rBV	30299	54231	8.89%	0.879%
21	8.637	2274	2285	2312	rBV2	241728	548395	89.93%	8.888%
22	8.788	2323	2332	2339	rBV	51509	82907	13.60%	1.344%
23	8.837	2339	2347	2376	rVB	113121	201492	33.04%	3.266%
24	9.418	2516	2528	2551	rBV	339167	588151	96.45%	9.532%
25	9.573	2567	2576	2589	rVB4	6023	9716	1.59%	0.157%
26	9.695	2603	2614	2631	rBV4	14316	26356	4.32%	0.427%
27	10.119	2729	2746	2769	rVB4	23776	58479	9.59%	0.948%
28	10.242	2775	2784	2797	rBV4	8158	14341	2.35%	0.232%
29	10.345	2800	2816	2830	rBV5	8014	19622	3.22%	0.318%
30	10.756	2932	2944	2958	rBV	108111	178268	29.23%	2.889%
31	11.476	3158	3168	3181	rBV6	7717	15443	2.53%	0.250%
32	11.689	3227	3234	3245	rBV6	9636	15335	2.51%	0.249%
33	11.814	3260	3273	3290	rBV	368521	609790	100.00%	9.883%
34	11.907	3295	3302	3316	rVB10	4697	7995	1.31%	0.130%
35	12.061	3339	3350	3375	rBV	66944	150625	24.70%	2.441%
36	12.193	3379	3391	3407	rVB	266967	440397	72.22%	7.137%

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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\SFAMUTR090123WMA.M
Title : TRACE VOA SFAM1.0

37	12.778	3565	3573	3583	rVB9	6246	10423	1.71%	0.169%
38	12.888	3598	3607	3620	rVB6	19864	32885	5.39%	0.533%
39	13.209	3699	3707	3717	rBV9	6046	10825	1.78%	0.175%
40	13.843	3898	3904	3914	rBV8	6093	10594	1.74%	0.172%
41	14.097	3971	3983	3995	rBV3	8723	15780	2.59%	0.256%
42	14.328	4048	4055	4063	rBV9	4738	6918	1.13%	0.112%

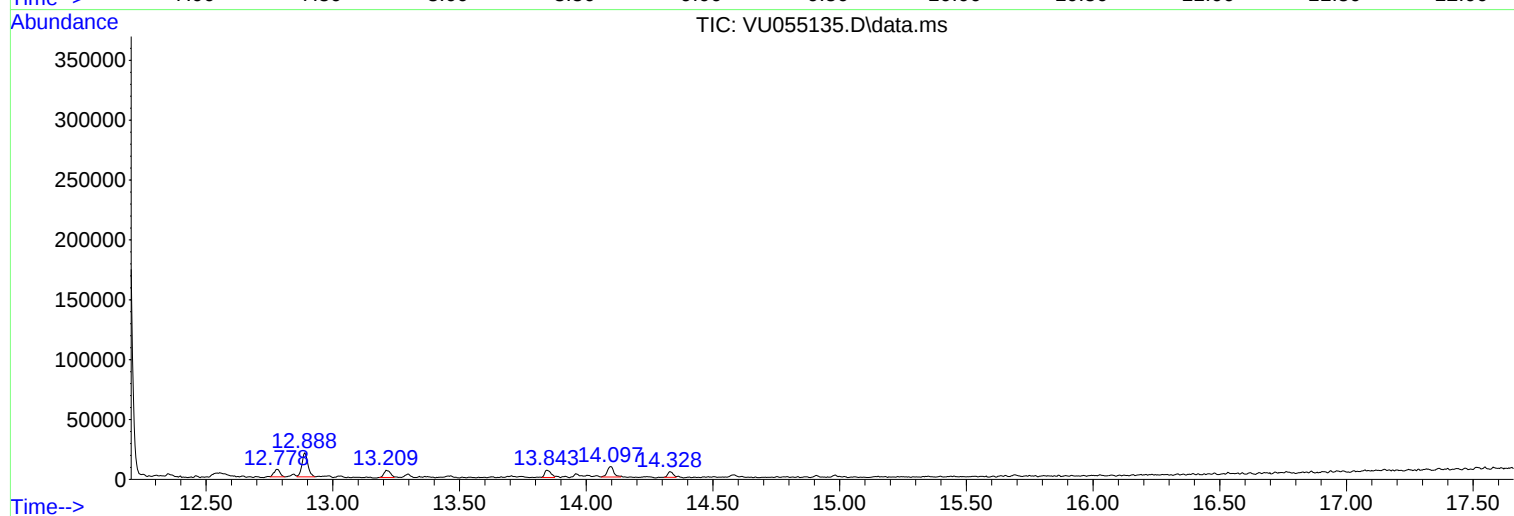
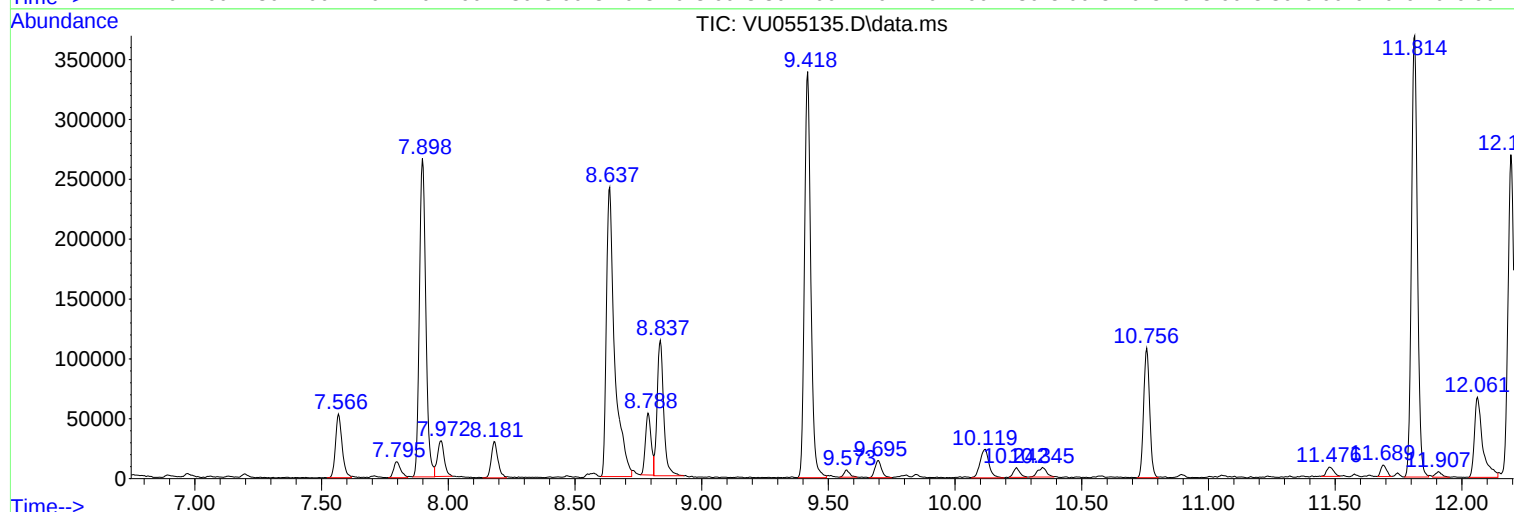
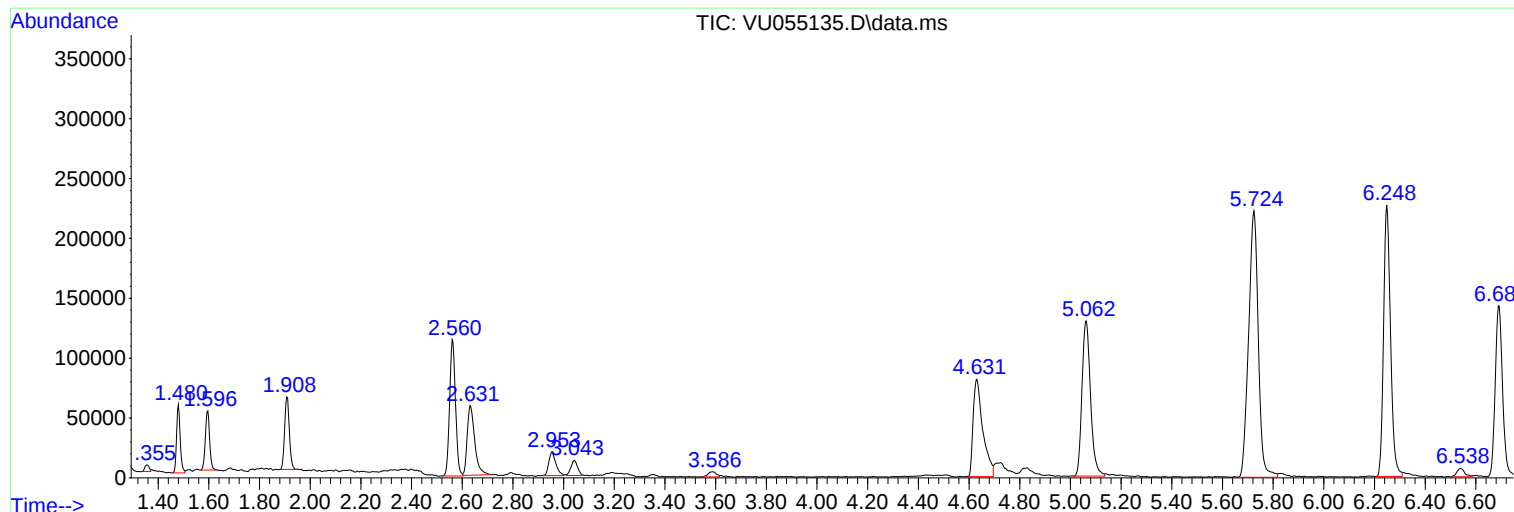
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH4F1

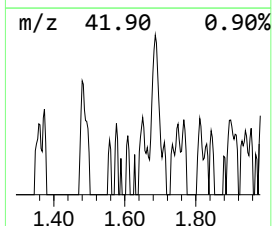
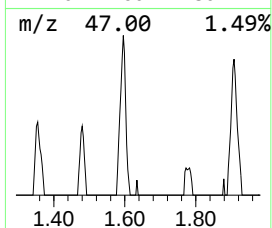
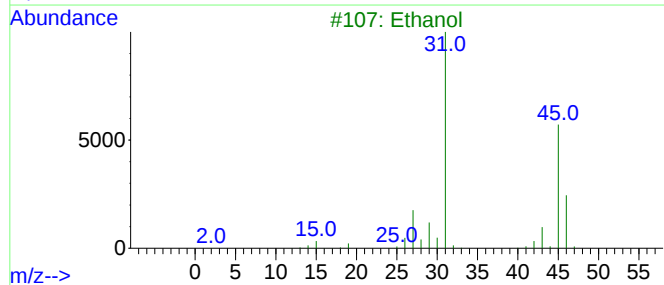
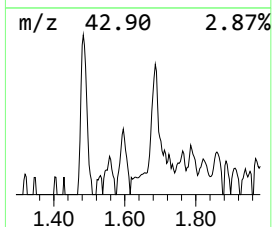
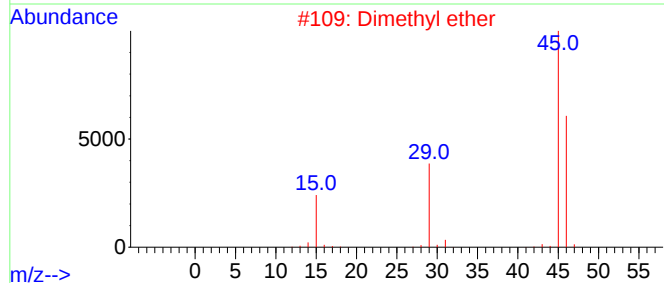
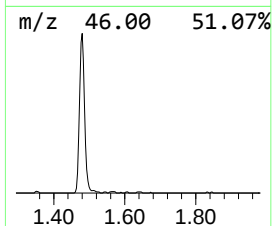
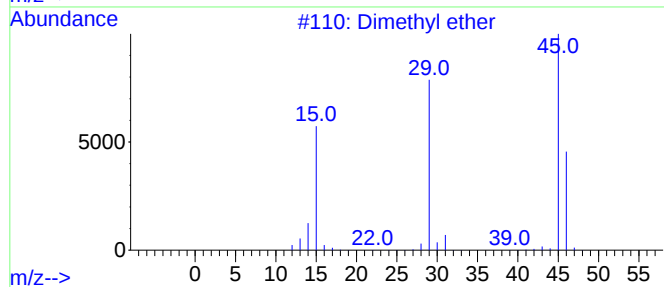
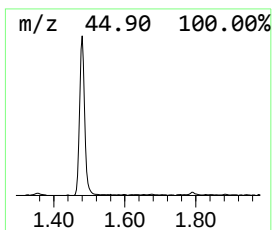
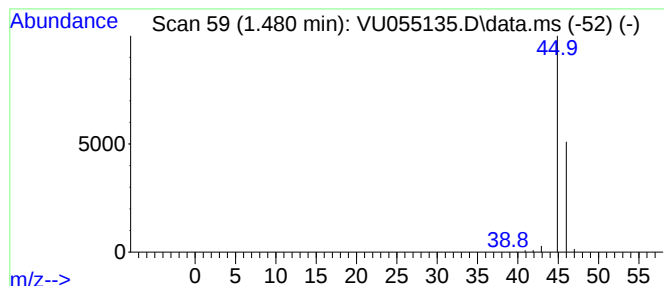
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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	0.66 ug/L	56999	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			Ethanol	46	C2H6O	000064-17-5	7
4			Dimethyl ether	46	C2H6O	000115-10-6	7
5			Ethanol	46	C2H6O	000064-17-5	7



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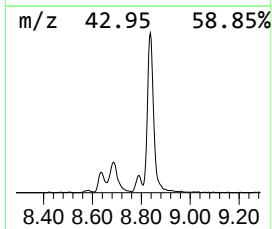
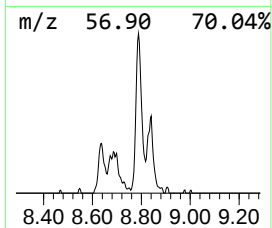
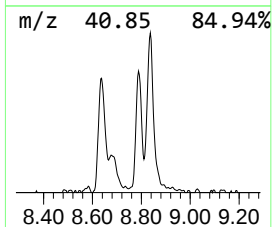
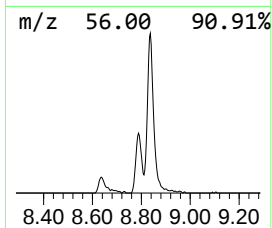
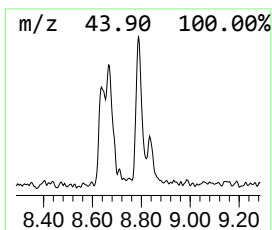
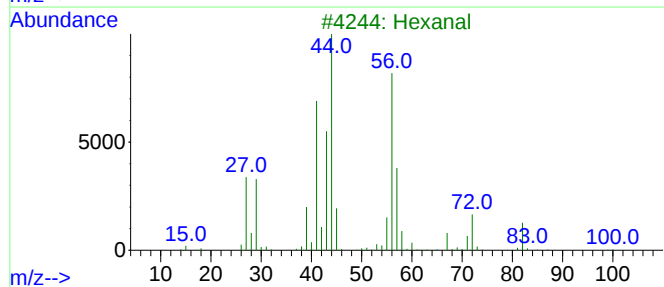
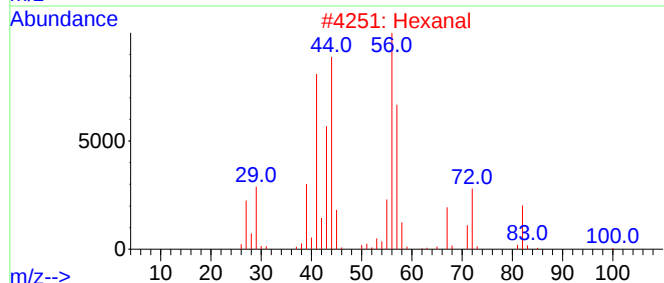
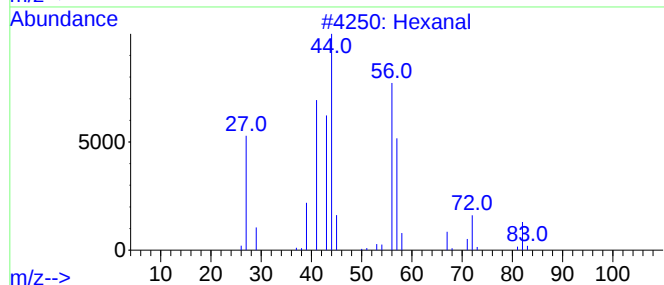
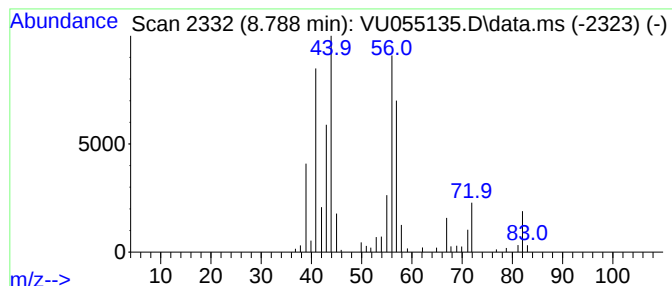
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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	0.70 ug/L	82907	Chlorobenzene-d5	9.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	72
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	59



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ALS Vial : 5 Sample Multiplier: 1

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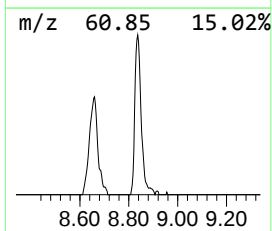
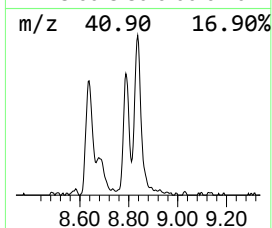
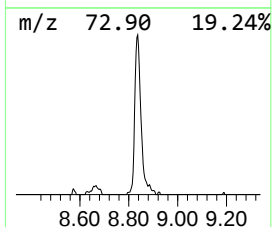
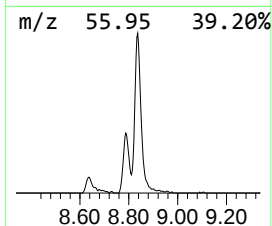
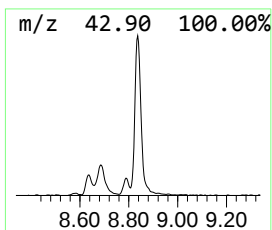
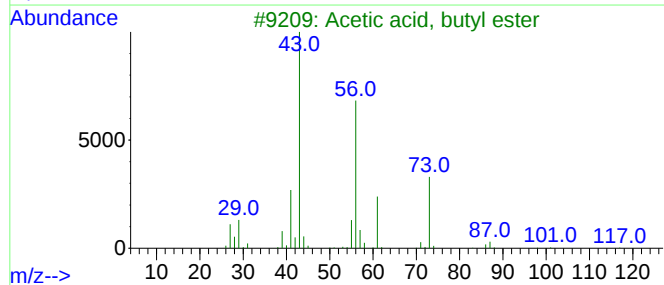
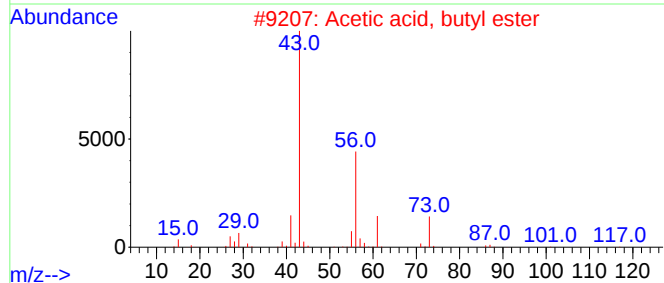
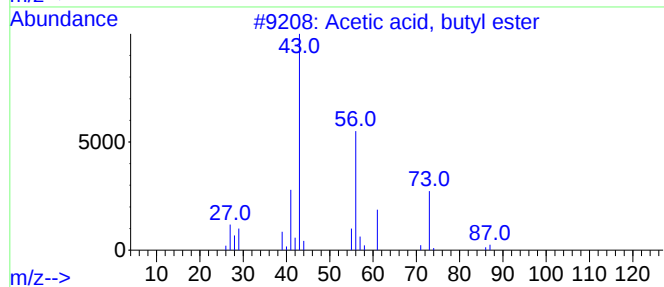
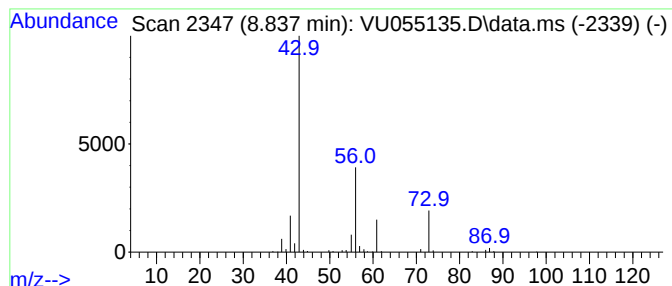
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
8.837	1.71 ug/L	201492	Chlorobenzene-d5	9.418

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	56	
4	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	43	
5	Isobutylamine		73	C4H11N	000078-81-9	9	



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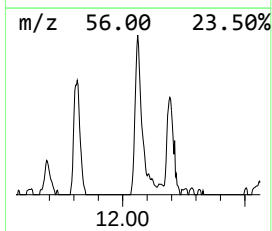
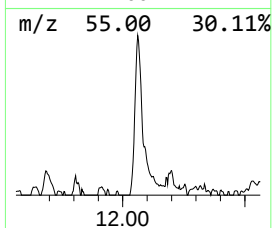
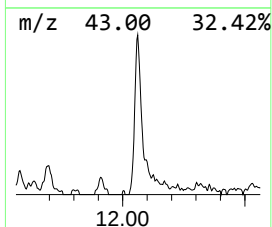
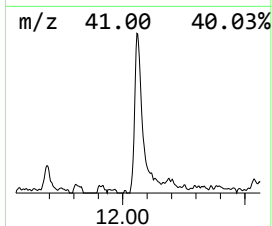
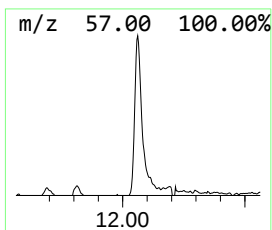
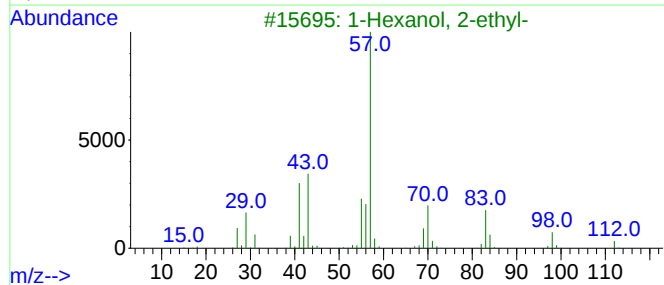
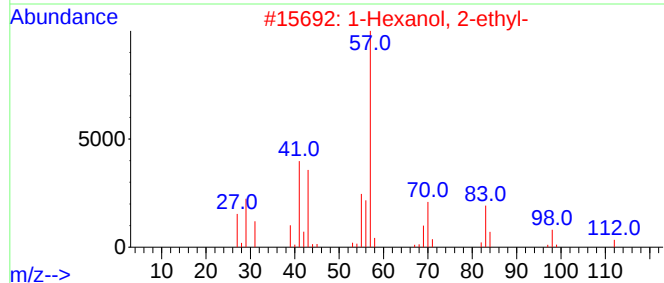
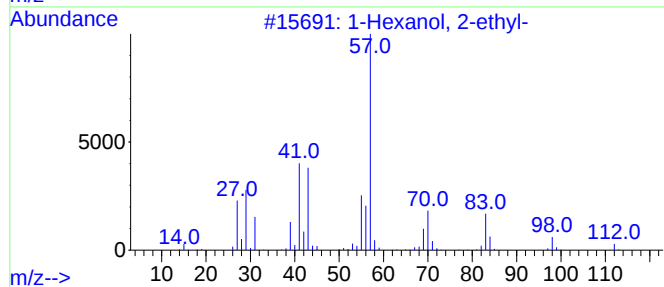
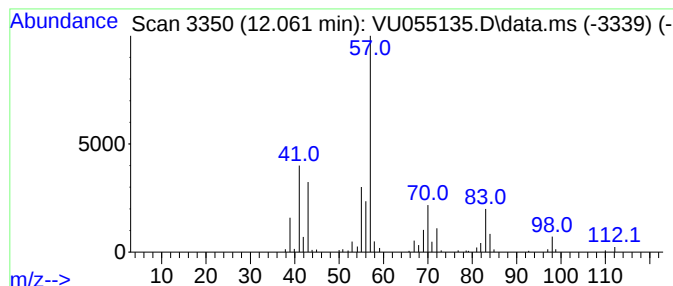
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.062	1.24 ug/L	150625	1,4-Dichlorobenzene-d4	11.814

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



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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	0.7	ug/L	56999	1	6.248	433634	5.0
Hexanal	8.788	0.7	ug/L	82907	2	9.418	588151	5.0
Acetic acid, bu...	8.837	1.7	ug/L	201492	2	9.418	588151	5.0
1-Hexanol, 2-et...	12.062	1.2	ug/L	150625	3	11.814	609790	5.0