

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080822\
 Data File : VU050195.D
 Acq On : 09 Aug 2022 21:55
 Operator : SY/MD
 Sample : N4115-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5E60

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\SFAMUTR080422WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU050195.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	70	80	93	rBV2	34505	40049	8.93%	1.228%
2	1.909	167	177	190	rVB	31282	40172	8.96%	1.232%
3	2.565	370	381	393	rBV	49095	78322	17.47%	2.401%
4	3.044	518	530	545	rVB2	23317	43380	9.67%	1.330%
5	4.623	1008	1021	1047	rBV	71602	180885	40.34%	5.546%
6	4.816	1069	1081	1094	rVB3	2967	6369	1.42%	0.195%
7	5.063	1144	1158	1179	rBV2	64368	146046	32.57%	4.478%
8	5.726	1340	1364	1387	rBV2	116483	314418	70.12%	9.640%
9	6.250	1514	1527	1544	rBV	95524	180242	40.20%	5.526%
10	6.530	1604	1614	1626	rVB3	7020	12608	2.81%	0.387%
11	6.694	1651	1665	1681	rBV2	83944	161476	36.01%	4.951%
12	7.568	1926	1937	1953	rBV3	32656	57119	12.74%	1.751%
13	7.899	2028	2040	2055	rBV	122279	209933	46.82%	6.436%
14	7.973	2055	2063	2072	rVB2	4139	7474	1.67%	0.229%
15	8.182	2117	2128	2146	rVB2	20057	34535	7.70%	1.059%
16	8.636	2256	2269	2298	rBV3	210284	448376	100.00%	13.747%
17	8.787	2306	2316	2325	rBV2	23755	38914	8.68%	1.193%
18	8.838	2325	2332	2344	rVB	7429	12268	2.74%	0.376%
19	9.417	2500	2512	2531	rBV	138328	233760	52.13%	7.167%
20	10.082	2707	2719	2740	rBV	12085	20525	4.58%	0.629%
21	10.218	2753	2761	2774	rBV5	3672	6920	1.54%	0.212%
22	10.758	2917	2929	2948	rVB	73566	117872	26.29%	3.614%
23	11.163	3048	3055	3063	rBV5	3723	6106	1.36%	0.187%
24	11.613	3186	3195	3208	rVB3	11968	17812	3.97%	0.546%
25	11.690	3212	3219	3224	rBV5	3386	5137	1.15%	0.157%
26	11.748	3224	3237	3244	rVV	38332	63102	14.07%	1.935%
27	11.812	3244	3257	3275	rVV2	136258	249410	55.63%	7.647%
28	11.915	3275	3289	3301	rVB4	39858	71870	16.03%	2.203%
29	12.063	3326	3335	3339	rBV3	12059	19355	4.32%	0.593%
30	12.195	3364	3376	3396	rVB	129861	209874	46.81%	6.434%
31	12.459	3447	3458	3466	rBV4	15263	22854	5.10%	0.701%
32	12.642	3502	3515	3527	rBV	5590	8295	1.85%	0.254%
33	12.841	3567	3577	3586	rBV	67504	104068	23.21%	3.191%
34	12.889	3586	3592	3602	rVB3	19000	29226	6.52%	0.896%
35	13.738	3847	3856	3867	rVB4	12668	20238	4.51%	0.620%
36	13.835	3878	3886	3896	rBV3	8851	13876	3.09%	0.425%

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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\SFAMUTR080422WMA.M
Title : TRACE VOA SFAM1.0

37	14.037	3938	3949	3960	rBV3	18457	28836	6.43%	0.884%
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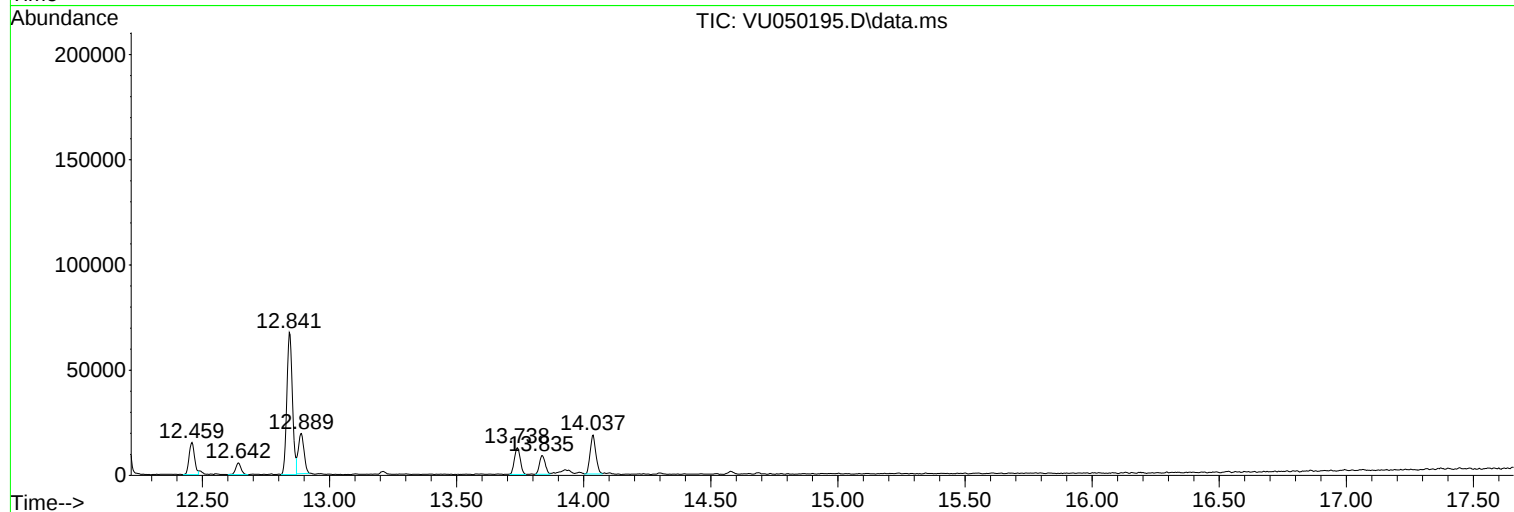
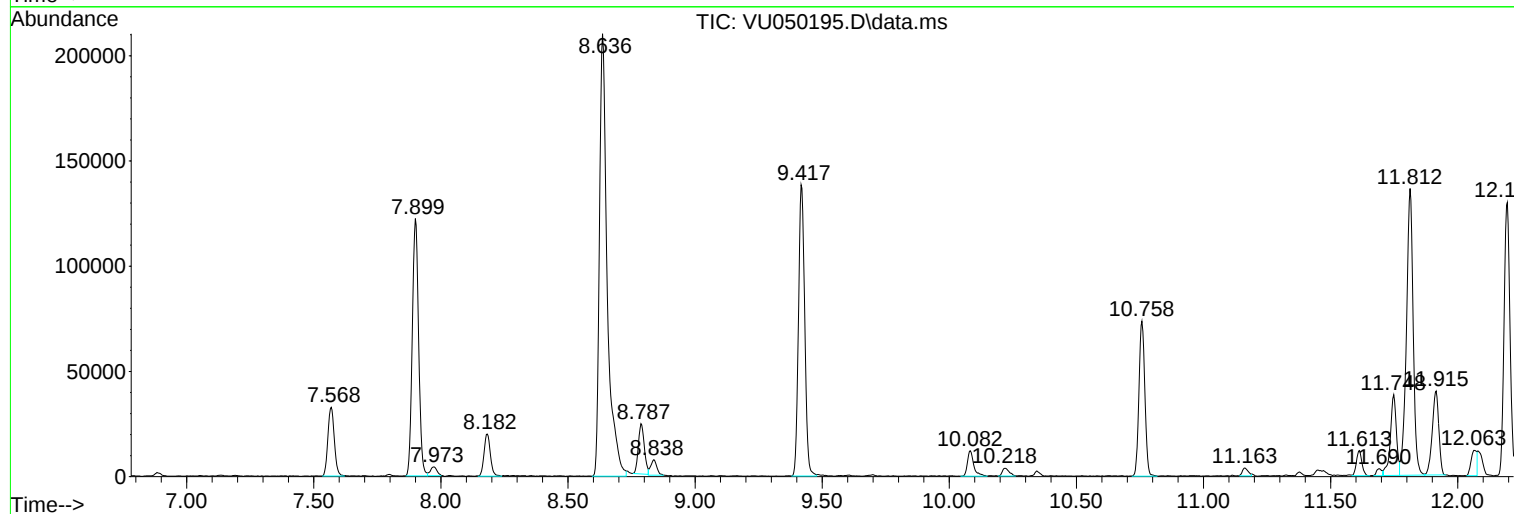
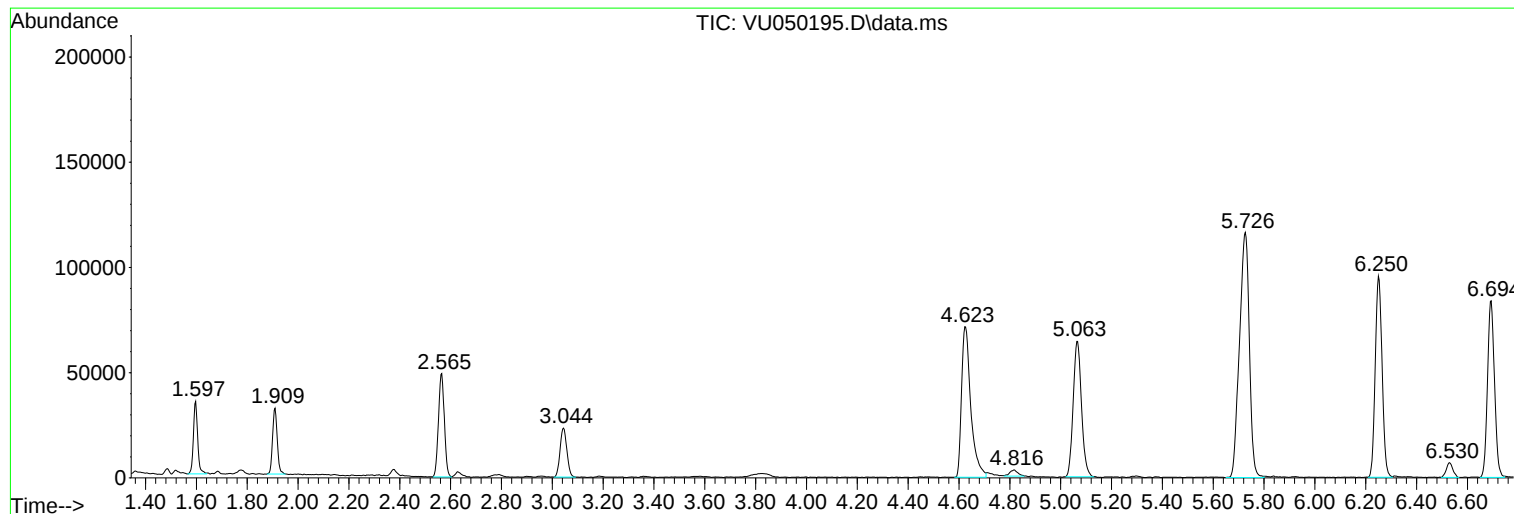
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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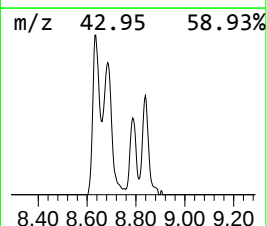
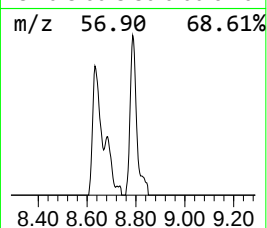
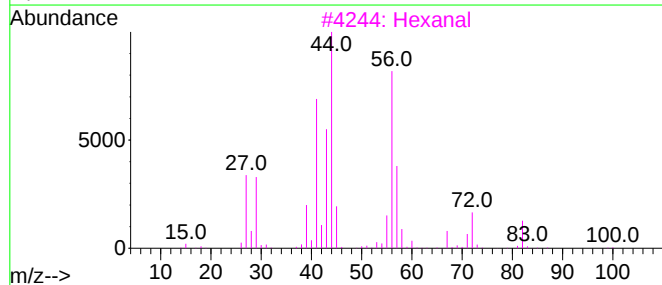
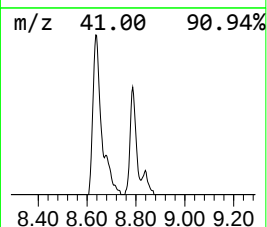
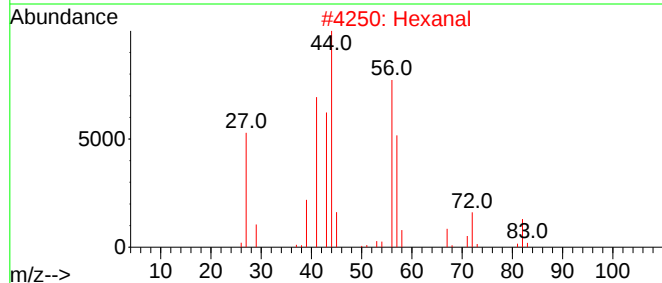
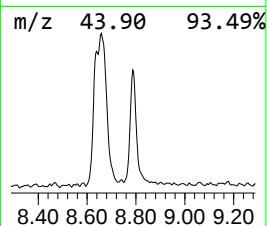
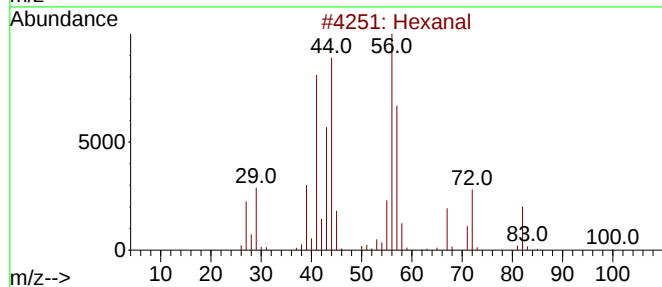
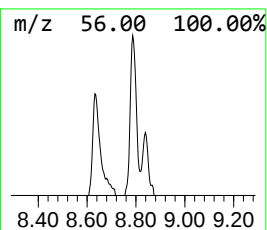
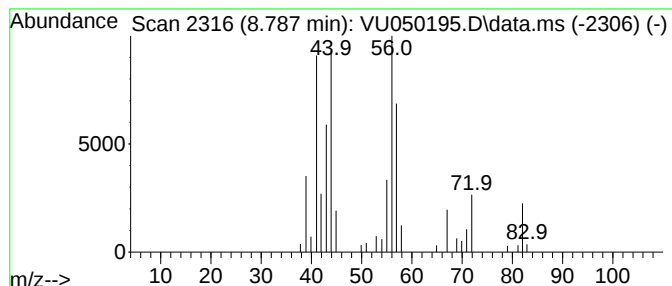
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	0.83 ug/L	38914	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	86
3	Hexanal			100	C6H12O	000066-25-1	78
4	Hexanal			100	C6H12O	000066-25-1	78
5	Hexanal			100	C6H12O	000066-25-1	72



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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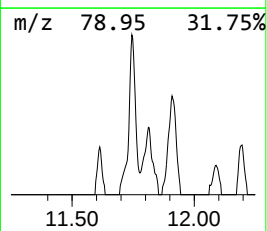
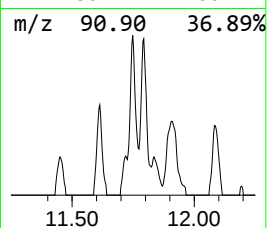
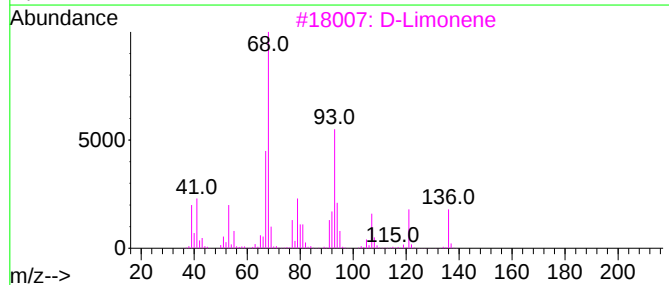
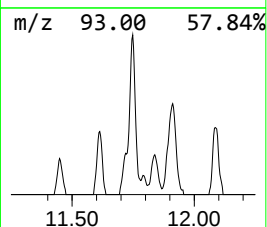
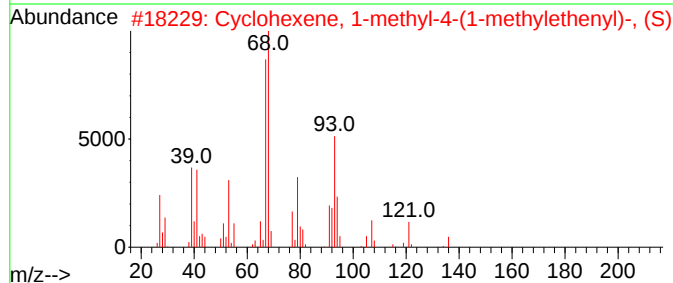
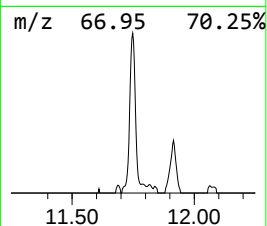
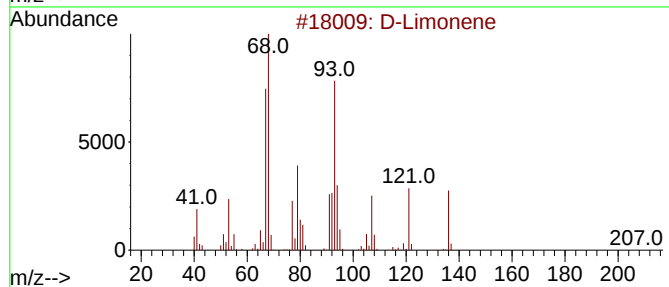
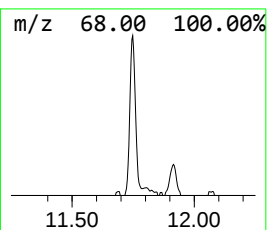
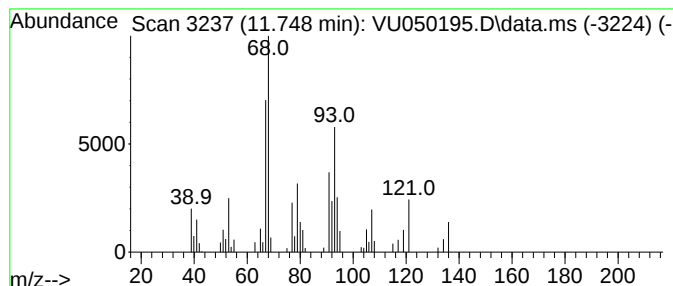
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 D-Limonene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.748	1.27 ug/L	63102	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	97
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	95
3			D-Limonene	136	C10H16	005989-27-5	91
4			D-Limonene	136	C10H16	005989-27-5	91
5			Limonene	136	C10H16	000138-86-3	90



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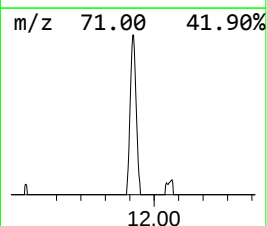
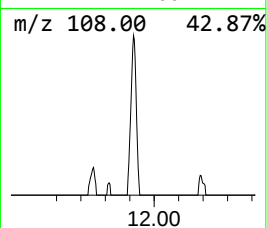
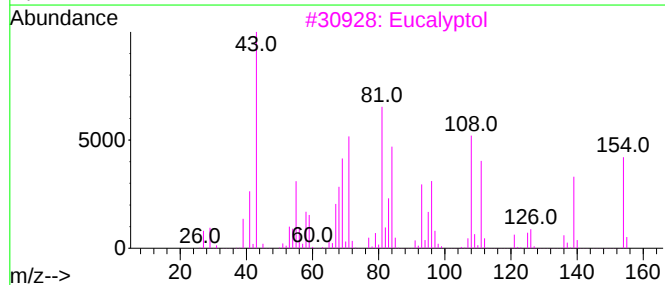
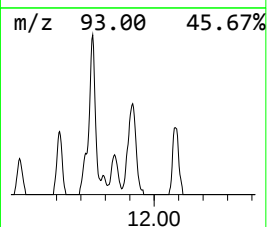
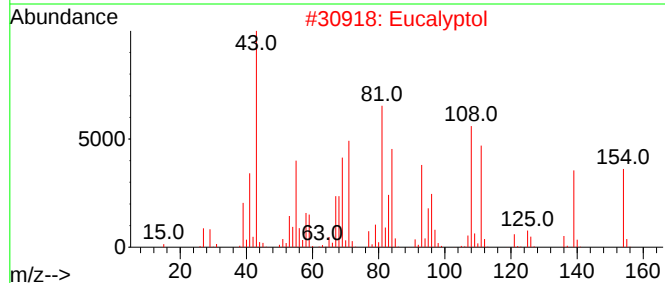
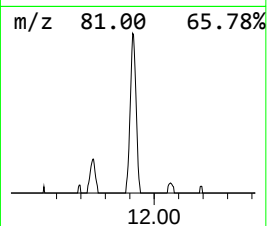
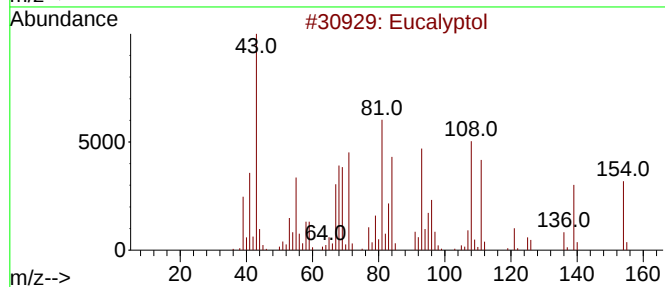
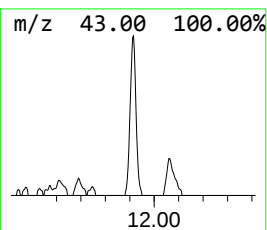
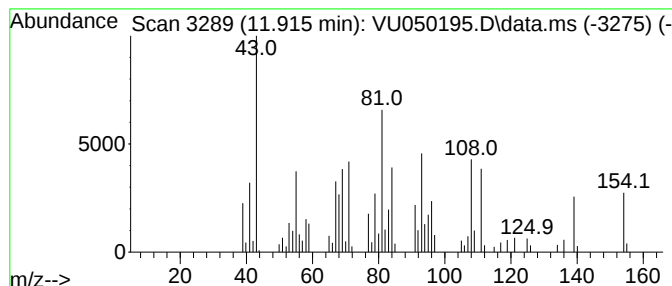
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Eucalyptol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.915	1.44 ug/L	71870	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol			154	C10H18O	000470-82-6	96
2	Eucalyptol			154	C10H18O	000470-82-6	96
3	Eucalyptol			154	C10H18O	000470-82-6	96
4	Eucalyptol			154	C10H18O	000470-82-6	94
5	Trifluoroacetyl-.alpha.-terpineol			250	C12H17F3O2	1000058-17-6	86



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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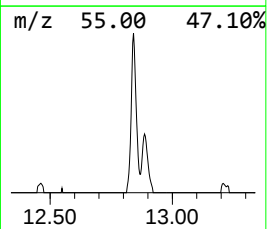
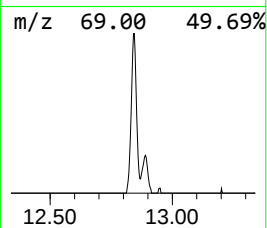
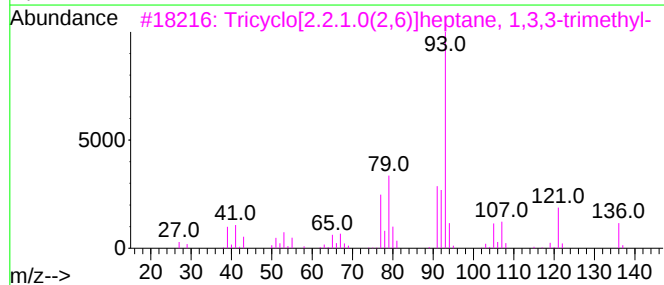
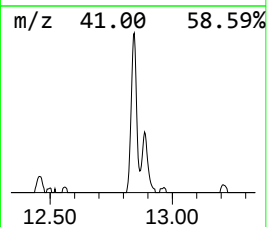
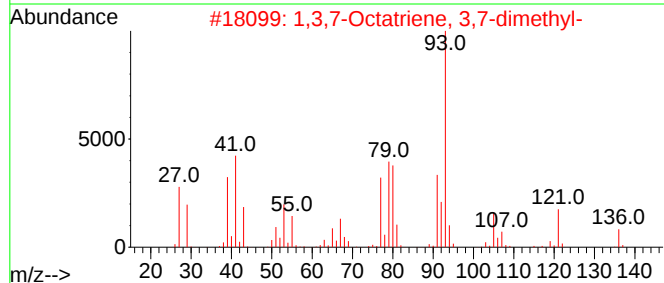
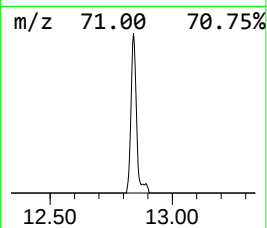
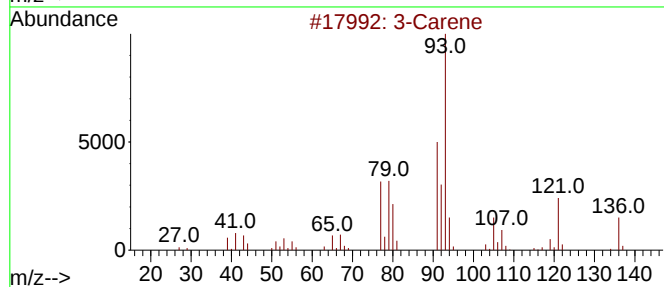
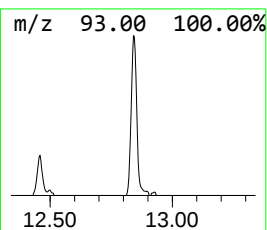
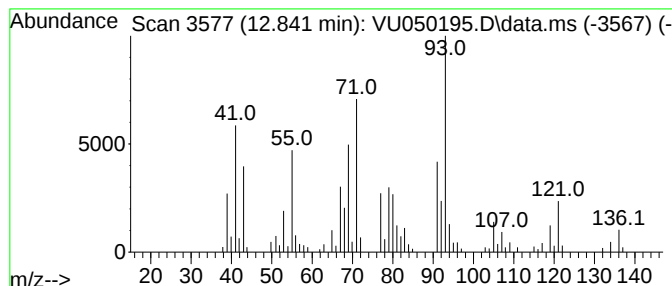
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 3-Carene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.841	2.09 ug/L	104068	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Carene	136	C10H16	013466-78-9	95
2			1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	93
3			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	92
4			1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	90
5			3-Carene	136	C10H16	013466-78-9	81



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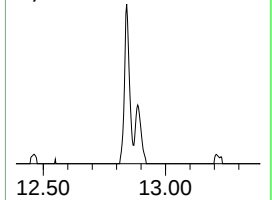
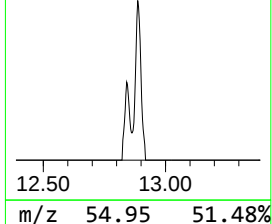
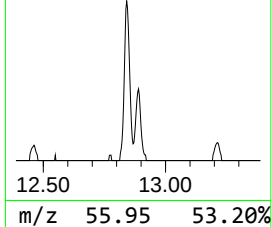
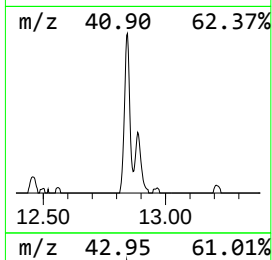
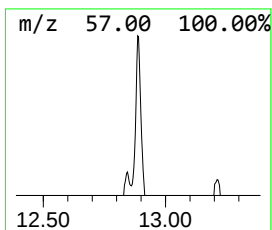
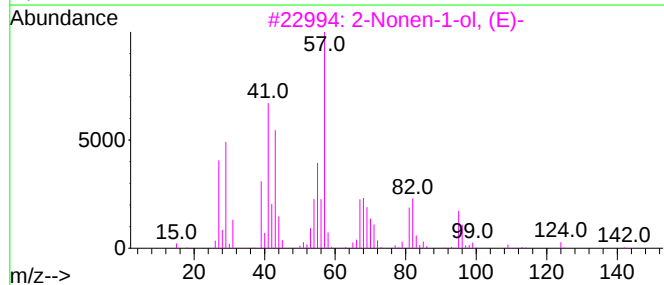
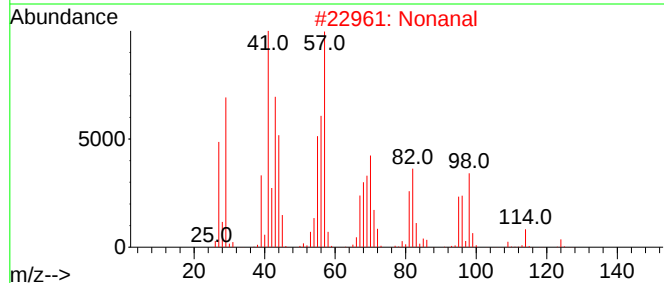
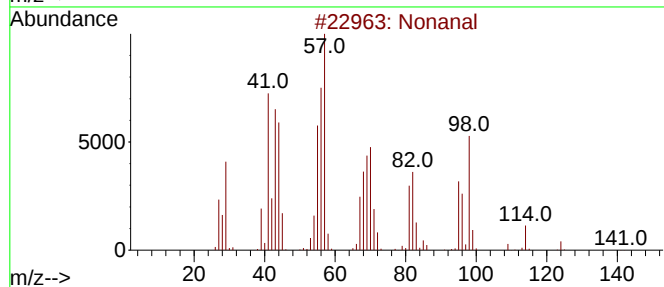
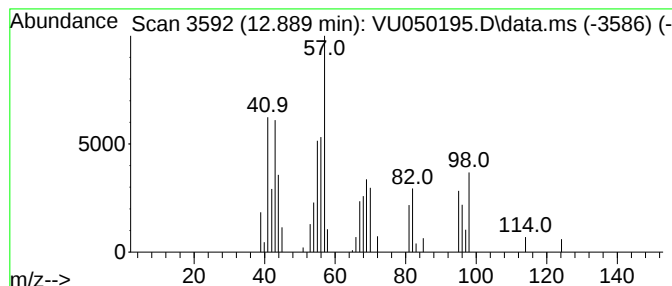
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Nonanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.889	0.59 ug/L	29226	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	86
2			Nonanal	142	C9H18O	000124-19-6	78
3			2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	43
4			2-Propenoic acid, undec-10-enyl ...	224	C14H24O2	020763-72-8	38
5			trans-2-Undecen-1-ol	170	C11H22O	075039-84-8	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080822\
Data File : VU050195.D
Acq On : 09 Aug 2022 21:55
Operator : SY/MD
Sample : N4115-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E60

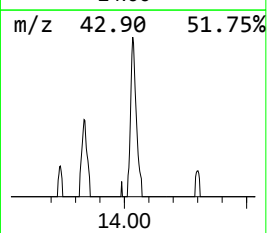
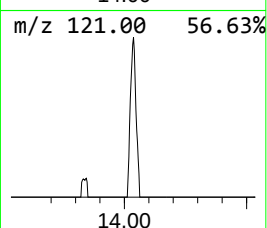
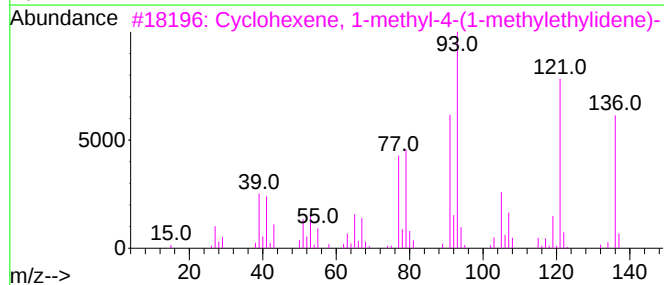
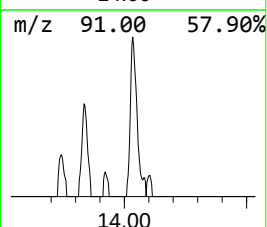
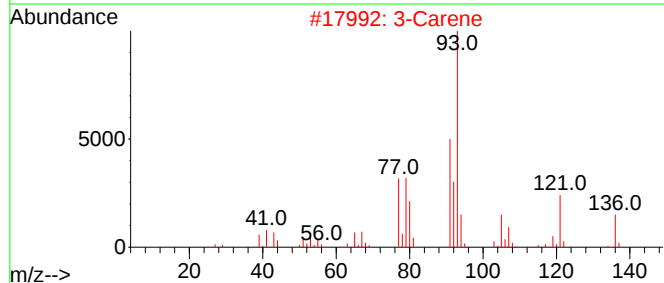
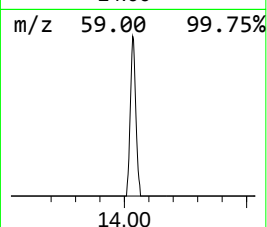
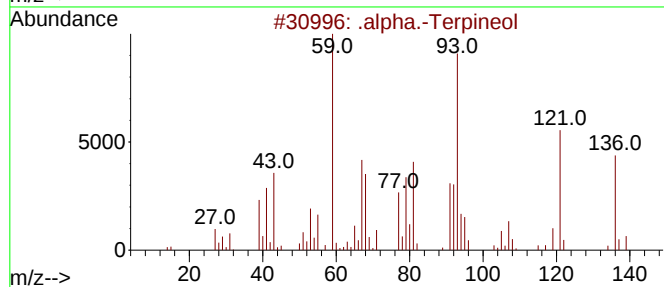
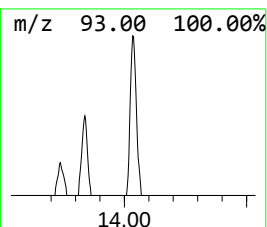
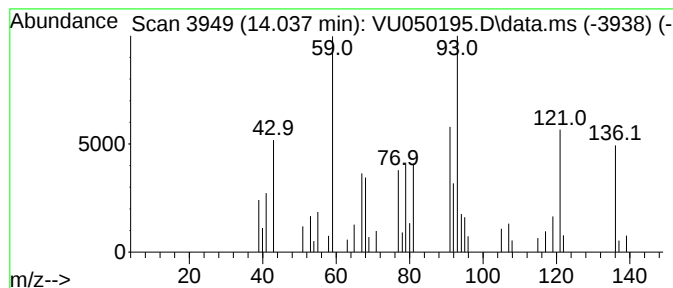
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 .alpha.-Terpineol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.037	0.58 ug/L	28836	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Terpineol	154	C10H18O	000098-55-5	91
2			3-Carene	136	C10H16	013466-78-9	83
3			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	64
4			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	64
5			Bicyclo[2.2.1]hept-2-ene, 1,7,7-...	136	C10H16	000464-17-5	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080822\
Data File : VU050195.D
Acq On : 09 Aug 2022 21:55
Operator : SY/MD
Sample : N4115-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.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
Hexanal	8.787	0.8	ug/L	38914	2	9.417	233760	5.0
D-Limonene	11.748	1.3	ug/L	63102	3	11.812	249410	5.0
Eucalyptol	11.915	1.4	ug/L	71870	3	11.812	249410	5.0
3-Carene	12.841	2.1	ug/L	104068	3	11.812	249410	5.0
Nonanal	12.889	0.6	ug/L	29226	3	11.812	249410	5.0
.alpha.-Terpineol	14.037	0.6	ug/L	28836	3	11.812	249410	5.0