

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081122\
 Data File : VU050300.D
 Acq On : 12 Aug 2022 23:21
 Operator : SY/MD
 Sample : N4115-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 37 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: VU050300.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.498	39	49	51	rBV4	10898	14854	3.73%	0.457%
2	1.597	73	80	92	rVB	43974	51043	12.82%	1.570%
3	1.909	170	177	194	rVB	39428	53602	13.46%	1.648%
4	2.565	369	381	393	rBV	61155	96983	24.36%	2.983%
5	2.626	393	400	414	rVB3	2617	4566	1.15%	0.140%
6	2.790	443	451	462	rVB	3354	5876	1.48%	0.181%
7	3.044	518	530	548	rVB	25577	46842	11.76%	1.441%
8	3.826	751	773	774	rBV	2317	4617	1.16%	0.142%
9	4.620	1008	1020	1045	rBV	67457	162853	40.90%	5.008%
10	4.809	1072	1079	1100	rVB3	3262	7009	1.76%	0.216%
11	5.063	1143	1158	1177	rBV2	65531	145912	36.65%	4.487%
12	5.726	1344	1364	1385	rBV2	120251	315944	79.35%	9.716%
13	6.250	1512	1527	1550	rBV	98912	187000	46.97%	5.751%
14	6.690	1651	1664	1684	rVB	83006	159145	39.97%	4.894%
15	7.565	1922	1936	1950	rBV	35202	60328	15.15%	1.855%
16	7.899	2027	2040	2054	rBV	125444	216126	54.28%	6.647%
17	7.970	2054	2062	2074	rVB2	4783	8274	2.08%	0.254%
18	8.179	2114	2127	2144	rVB	21509	35534	8.92%	1.093%
19	8.632	2256	2268	2301	rBV3	193541	398161	100.00%	12.245%
20	8.787	2306	2316	2325	rVV3	21353	36511	9.17%	1.123%
21	8.835	2325	2331	2347	rVB2	7885	13524	3.40%	0.416%
22	9.417	2500	2512	2532	rBV	142647	237020	59.53%	7.289%
23	10.079	2706	2718	2728	rBV2	12880	20083	5.04%	0.618%
24	10.218	2751	2761	2773	rBV4	4335	7426	1.87%	0.228%
25	10.758	2916	2929	2943	rBV	70040	111097	27.90%	3.417%
26	11.610	3186	3194	3205	rBV2	17892	26430	6.64%	0.813%
27	11.690	3210	3219	3224	rBV4	4308	7066	1.77%	0.217%
28	11.745	3226	3236	3244	rVV2	41172	66918	16.81%	2.058%
29	11.812	3244	3257	3273	rVV2	146586	286774	72.02%	8.819%
30	11.912	3276	3288	3307	rVB2	44223	76164	19.13%	2.342%
31	12.063	3325	3335	3338	rBV3	14055	19215	4.83%	0.591%
32	12.192	3363	3375	3397	rVB	125347	206371	51.83%	6.347%
33	12.455	3449	3457	3466	rBV5	11717	18062	4.54%	0.555%
34	12.639	3506	3514	3525	rBV2	8917	12429	3.12%	0.382%
35	12.841	3568	3577	3585	rBV3	26203	39754	9.98%	1.223%
36	12.886	3585	3591	3601	rVB4	21044	30903	7.76%	0.950%

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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	13.211	3684	3692	3701	rVB2	3038	4262	1.07%	0.131%
38	13.738	3847	3856	3867	rVB4	12157	19358	4.86%	0.595%
39	13.835	3878	3886	3896	rBV7	8246	15638	3.93%	0.481%
40	14.034	3940	3948	3962	rBV5	13271	21981	5.52%	0.676%

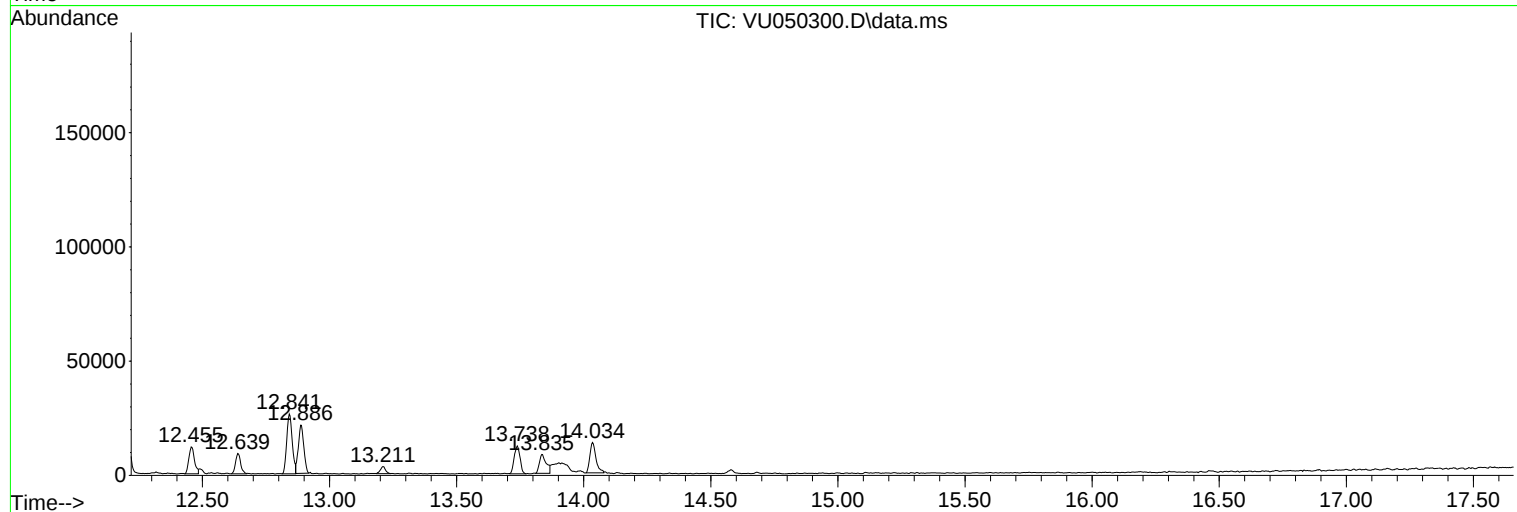
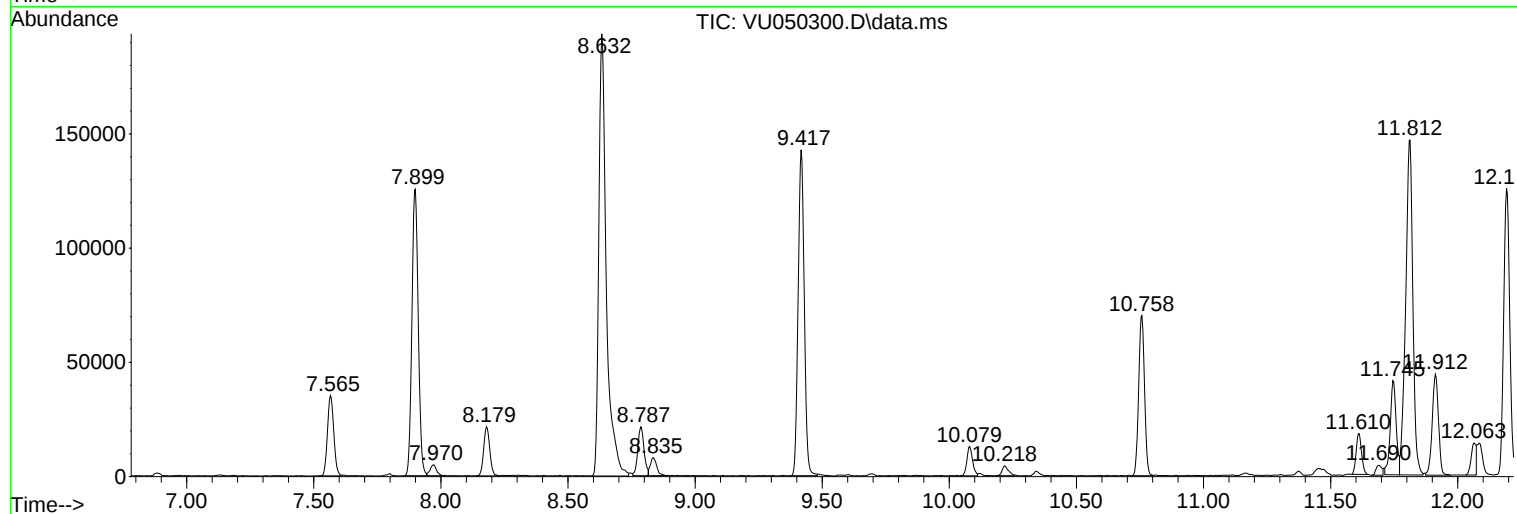
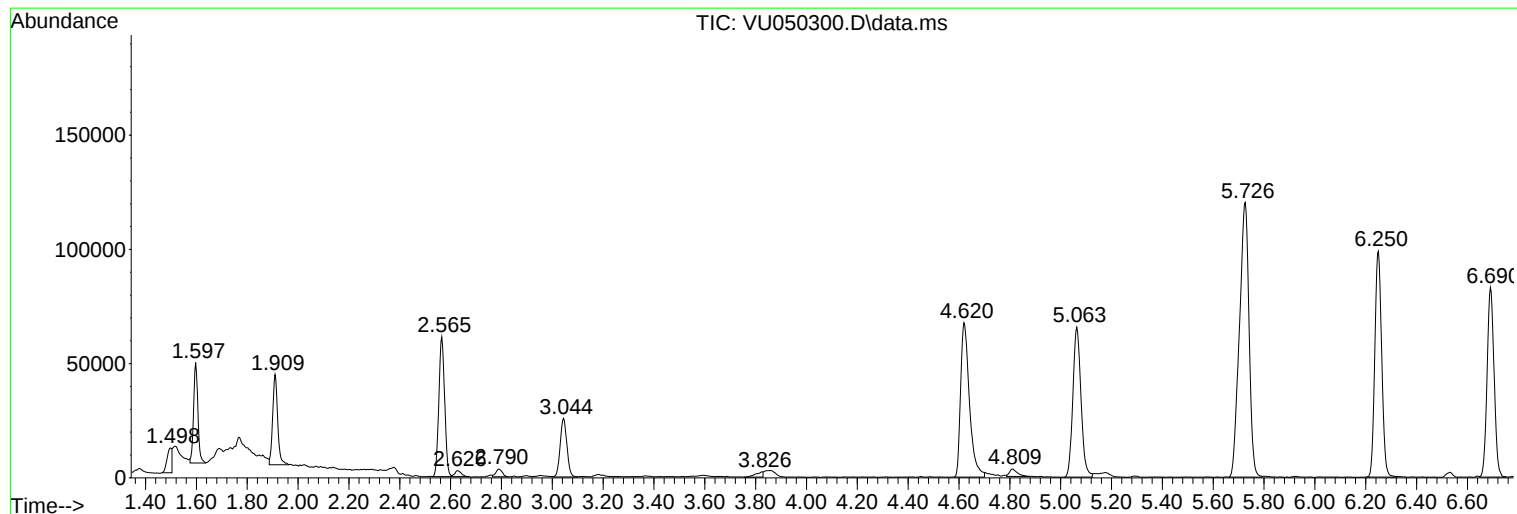
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Misc : 25.0mL/MSVOA_U/WATER
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Instrument :
MSVOA_U
ClientSampleId :
F5E60

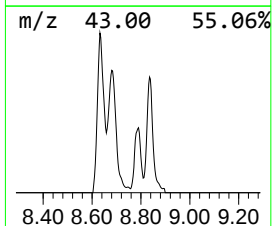
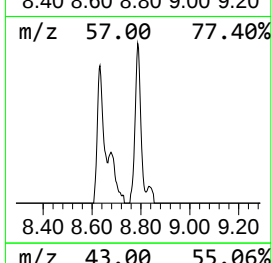
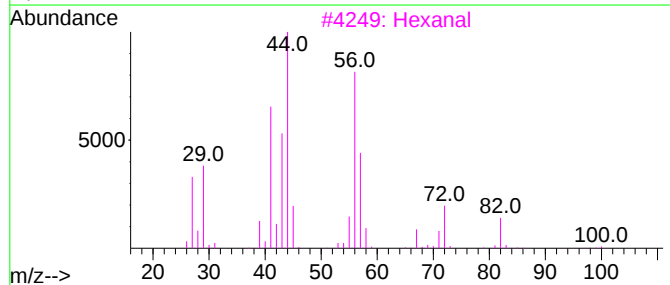
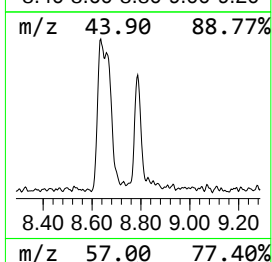
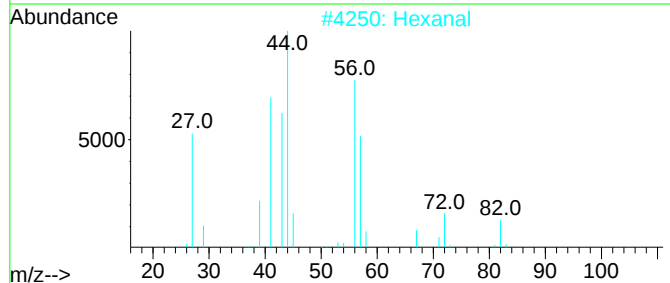
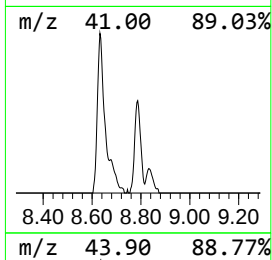
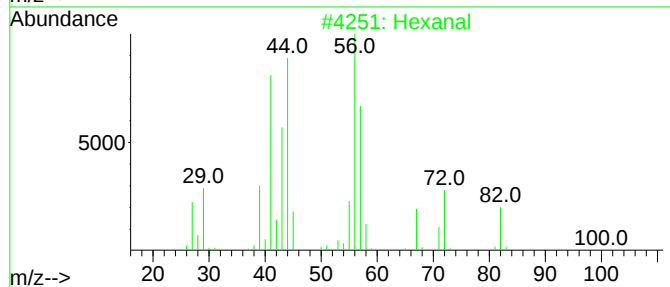
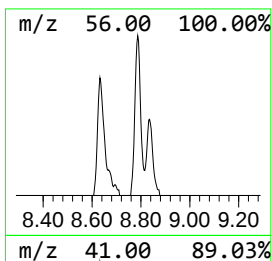
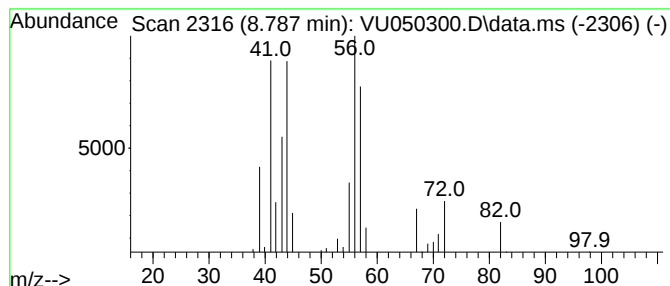
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	0.77 ug/L	36511	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	59
4	Hexanal			100	C6H12O	000066-25-1	45
5	Hexanal			100	C6H12O	000066-25-1	45



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ALS Vial : 37 Sample Multiplier: 1

Instrument :
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ClientSampleId :
F5E60

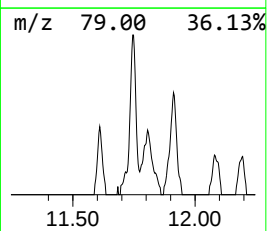
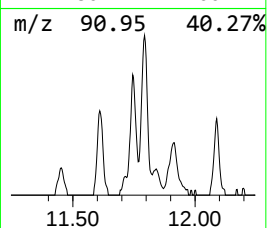
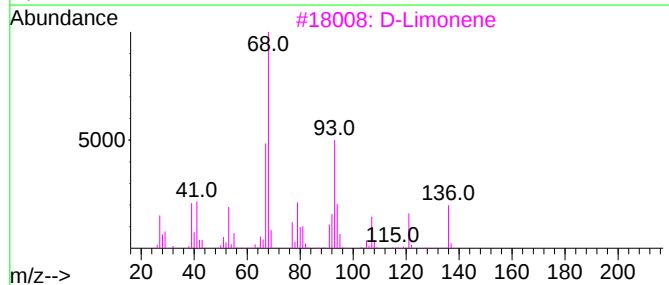
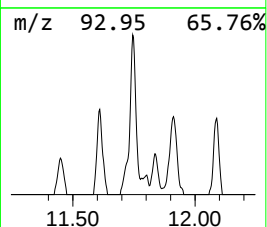
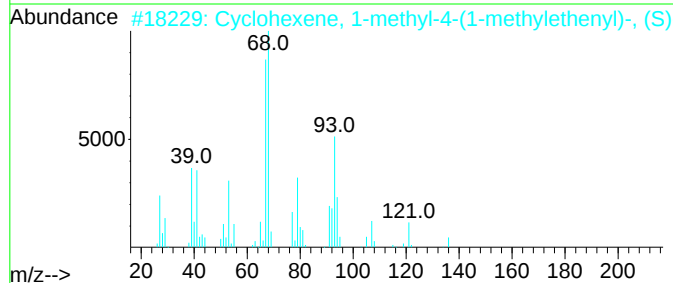
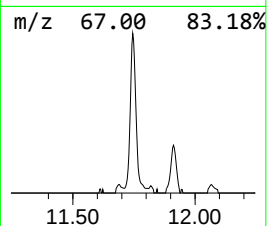
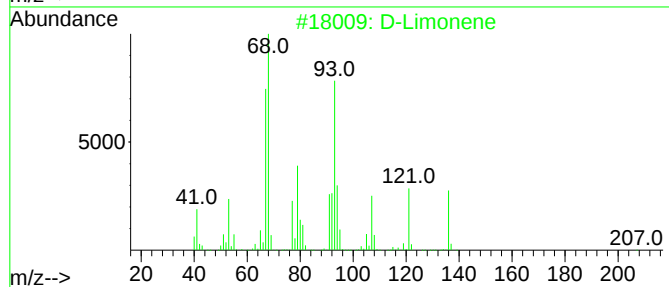
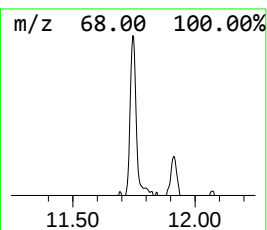
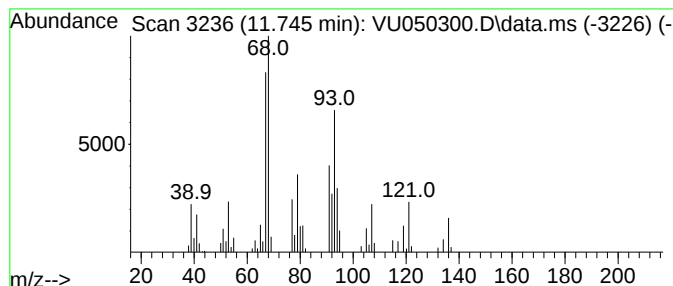
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 D-Limonene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	1.17 ug/L	66918	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	98
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	97
3			D-Limonene	136	C10H16	005989-27-5	93
4			D-Limonene	136	C10H16	005989-27-5	90
5			D-Limonene	136	C10H16	005989-27-5	81



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 37 Sample Multiplier: 1

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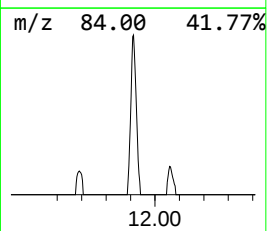
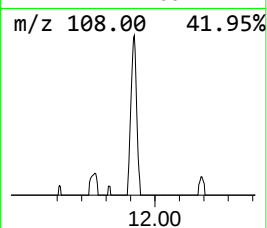
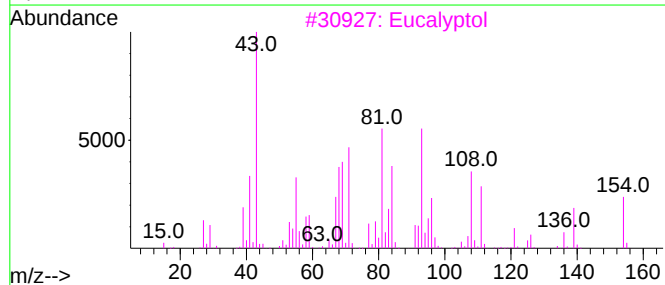
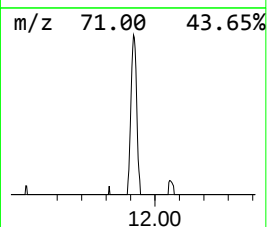
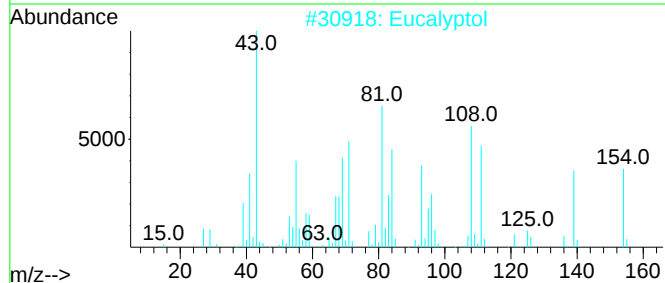
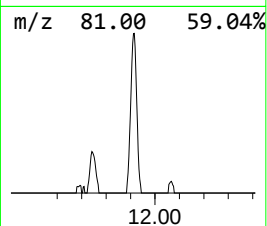
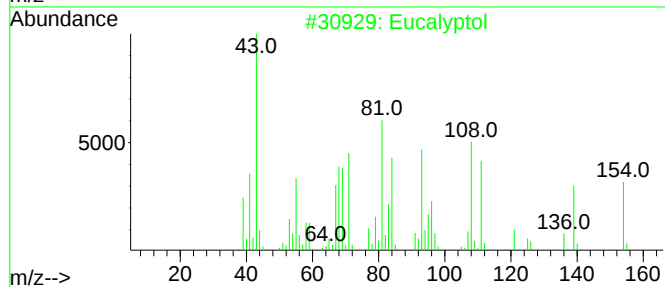
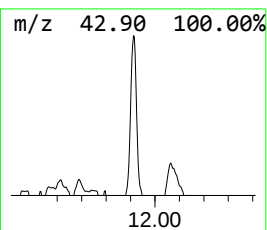
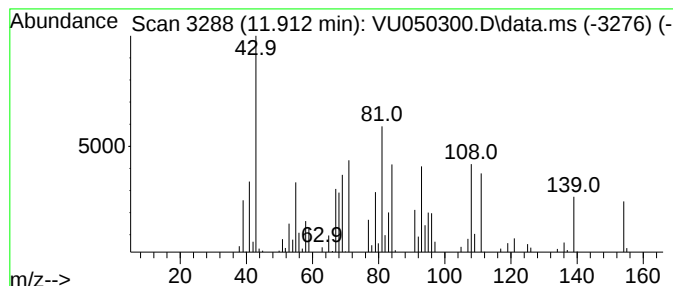
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Eucalyptol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.912	1.33 ug/L	76164	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol			154	C10H18O	000470-82-6	98
2	Eucalyptol			154	C10H18O	000470-82-6	97
3	Eucalyptol			154	C10H18O	000470-82-6	93
4	Eucalyptol			154	C10H18O	000470-82-6	90
5	Eucalyptol			154	C10H18O	000470-82-6	76



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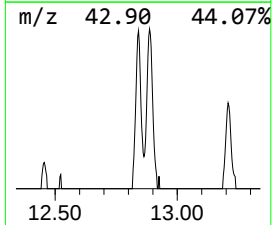
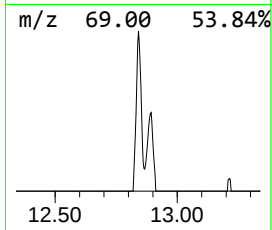
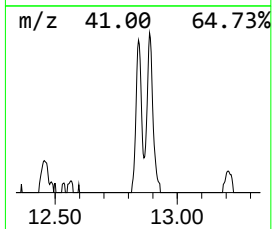
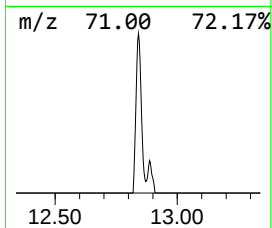
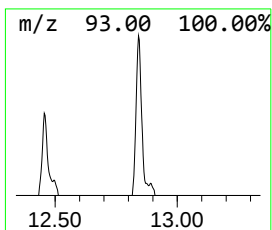
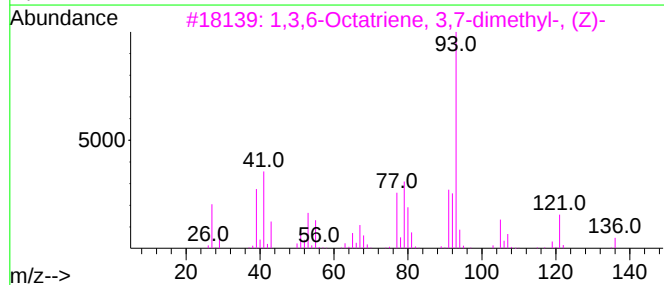
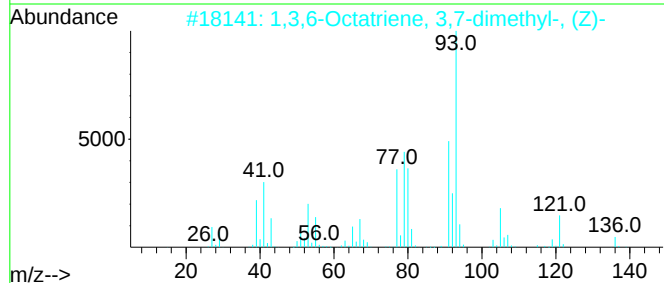
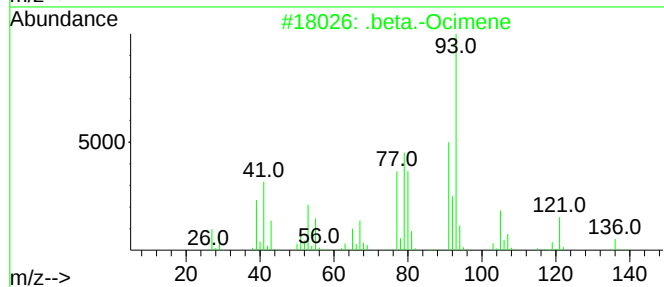
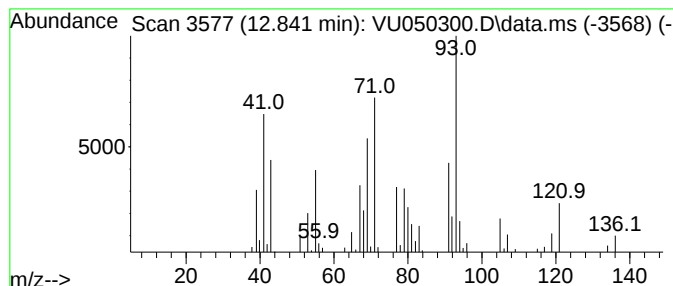
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 .beta.-Ocimene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.841	0.69 ug/L	39754	1,4-Dichlorobenzene-d4	11.812	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Ocimene	136	C10H16	013877-91-3	94
2	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	81
3	1,3,6-Octatriene, 3,7-dimethyl-,...	136	C10H16	003338-55-4	70
4	1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	70
5	Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	64



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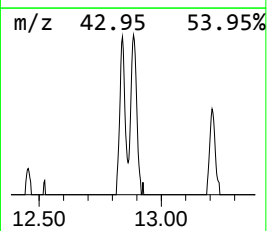
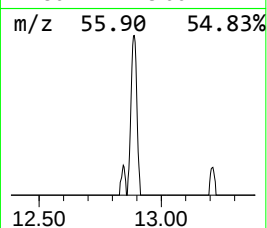
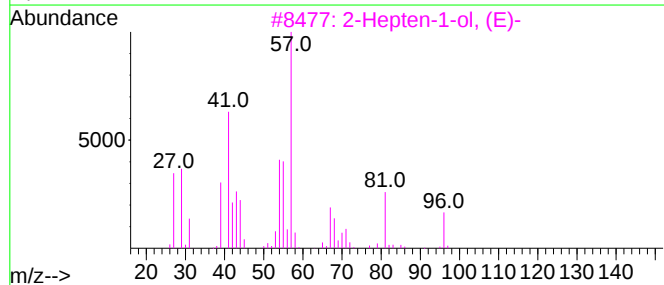
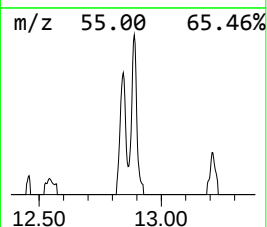
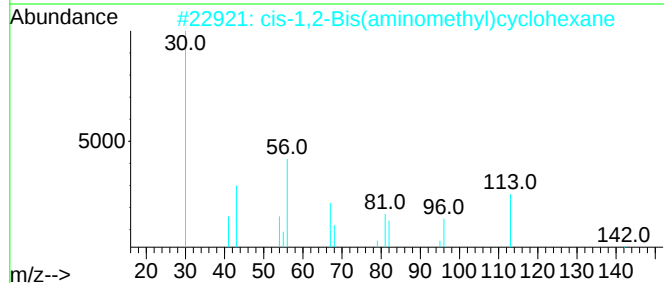
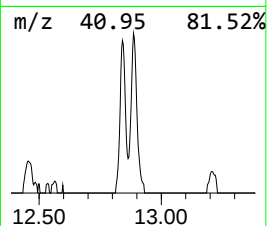
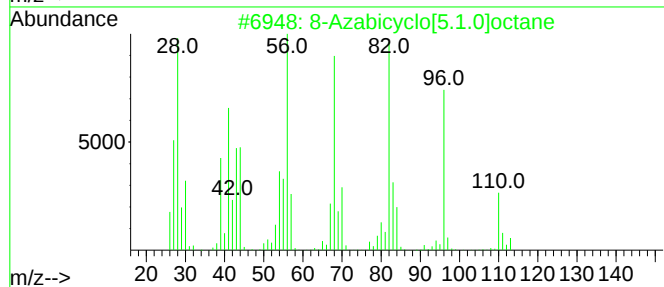
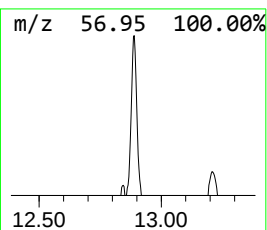
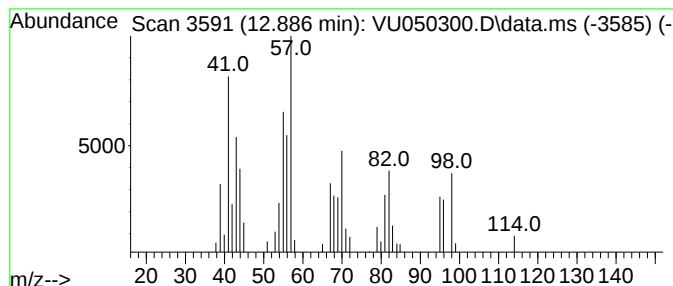
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	0.54 ug/L	30903	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			8-Azabicyclo[5.1.0]octane	111	C7H13N	000286-44-2	35
2			cis-1,2-Bis(aminomethyl)cyclohexane	142	C8H18N2	070795-45-8	22
3			2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	22
4			3-Hepten-1-ol, (E)-	114	C7H14O	002108-05-6	18
5			Nonamethylene glycol	204	C11H24O3	1000129-54-8	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081122\
Data File : VU050300.D
Acq On : 12 Aug 2022 23:21
Operator : SY/MD
Sample : N4115-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 37 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	36511	2	9.417	237020	5.0
D-Limonene	11.745	1.2	ug/L	66918	3	11.812	286774	5.0
Eucalyptol	11.912	1.3	ug/L	76164	3	11.812	286774	5.0
.beta.-Ocimene	12.841	0.7	ug/L	39754	3	11.812	286774	5.0
unknown-01	12.886	0.5	ug/L	30903	3	11.812	286774	5.0