

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
 Data File : VU050089.D
 Acq On : 05 Aug 2022 11:38
 Operator : SY/MD
 Sample : N4022-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5E53

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: VU050089.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	70	79	95	rBV	43647	50885	12.58%	1.479%
2	1.909	169	177	193	rVB	38201	48598	12.01%	1.413%
3	2.565	367	381	396	rVB	67610	107454	26.56%	3.124%
4	3.044	518	530	546	rVB	31173	57825	14.29%	1.681%
5	4.633	1012	1024	1068	rBV	55773	165783	40.98%	4.820%
6	4.816	1072	1081	1096	rVB3	2618	5913	1.46%	0.172%
7	5.064	1140	1158	1181	rBV	64507	147707	36.51%	4.294%
8	5.726	1344	1364	1387	rBV2	130349	339416	83.89%	9.867%
9	6.250	1514	1527	1544	rBV	92651	173592	42.91%	5.047%
10	6.690	1650	1664	1683	rBV	82736	160790	39.74%	4.674%
11	7.568	1926	1937	1954	rBV	39364	69551	17.19%	2.022%
12	7.899	2027	2040	2055	rBV	149390	260424	64.37%	7.571%
13	7.970	2056	2062	2077	rVB	4691	8625	2.13%	0.251%
14	8.182	2117	2128	2146	rBV	24691	42599	10.53%	1.238%
15	8.639	2258	2270	2304	rBV4	169082	404579	100.00%	11.762%
16	8.790	2307	2317	2326	rVV2	30049	53451	13.21%	1.554%
17	8.835	2326	2331	2356	rVB2	8078	15912	3.93%	0.463%
18	9.420	2500	2513	2541	rBV	130134	219239	54.19%	6.374%
19	10.083	2709	2719	2737	rBV3	12285	23816	5.89%	0.692%
20	10.221	2753	2762	2776	rBV3	5547	9964	2.46%	0.290%
21	10.758	2918	2929	2943	rBV	72498	115031	28.43%	3.344%
22	11.163	3046	3055	3063	rBV2	6458	10294	2.54%	0.299%
23	11.378	3114	3122	3129	rBV3	4008	5469	1.35%	0.159%
24	11.452	3136	3145	3147	rBV4	4456	5383	1.33%	0.156%
25	11.613	3186	3195	3206	rVB3	12884	17981	4.44%	0.523%
26	11.700	3211	3222	3223	rBV5	3860	5369	1.33%	0.156%
27	11.716	3223	3227	3229	rVV2	5986	6368	1.57%	0.185%
28	11.748	3229	3237	3245	rVV	37974	61894	15.30%	1.799%
29	11.812	3245	3257	3275	rVV2	132439	242890	60.04%	7.061%
30	11.915	3275	3289	3303	rVB4	47821	88122	21.78%	2.562%
31	12.063	3325	3335	3340	rBV2	13329	22776	5.63%	0.662%
32	12.195	3364	3376	3397	rBV	139162	229358	56.69%	6.668%
33	12.459	3448	3458	3473	rBV2	19255	29968	7.41%	0.871%
34	12.642	3508	3515	3528	rVB5	3298	4748	1.17%	0.138%
35	12.841	3567	3577	3586	rBV	90293	143811	35.55%	4.181%
36	12.890	3586	3592	3609	rVB2	19238	30257	7.48%	0.880%

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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	3702	rBV5	3278	5001	1.24%	0.145%
38	13.738	3847	3856	3868	rVB4	12131	19685	4.87%	0.572%
39	13.838	3876	3887	3897	rBV5	10829	16106	3.98%	0.468%
40	14.037	3940	3949	3957	rBV6	8532	13146	3.25%	0.382%

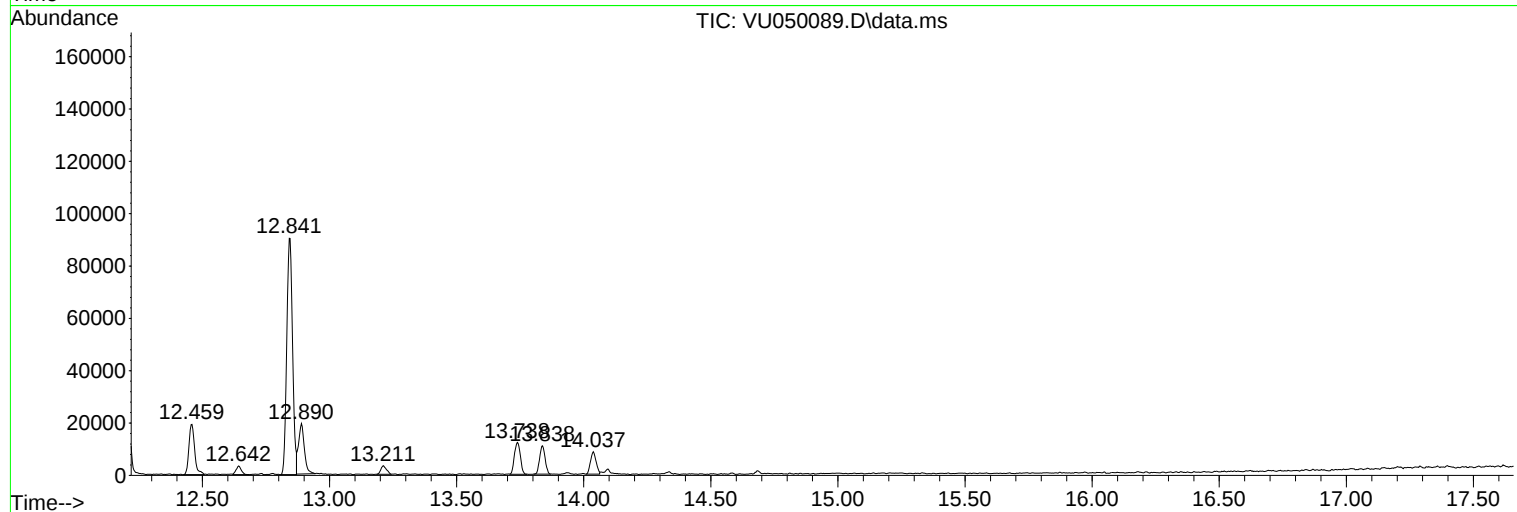
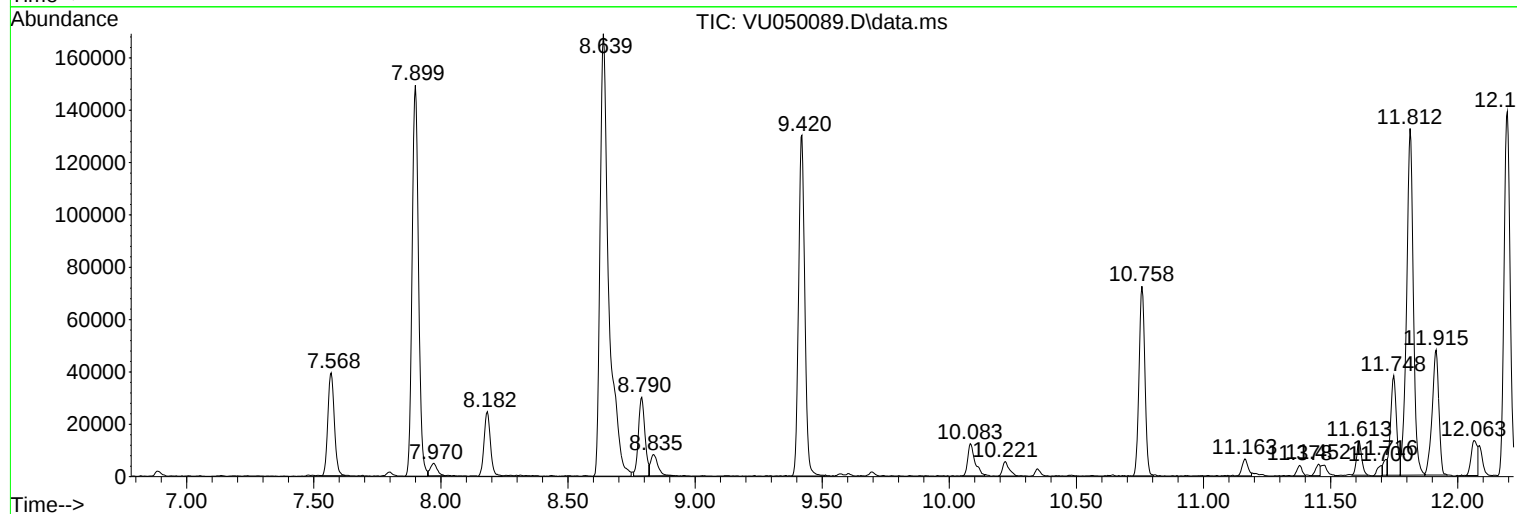
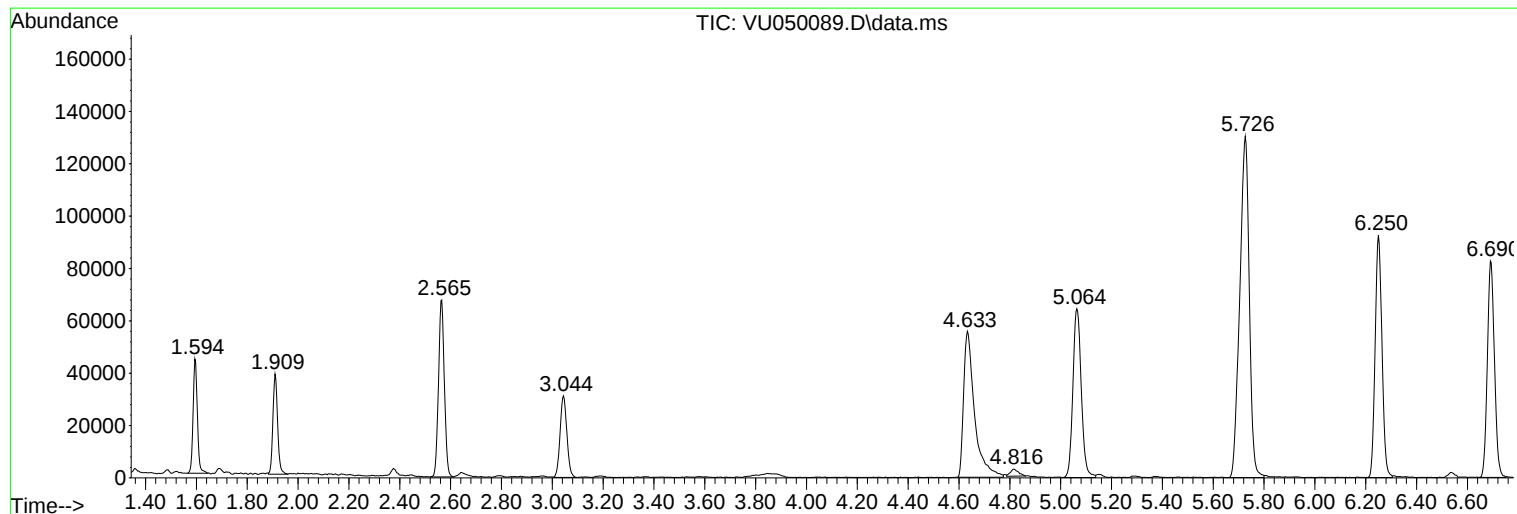
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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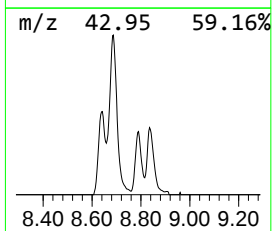
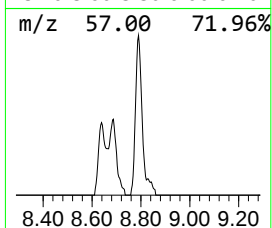
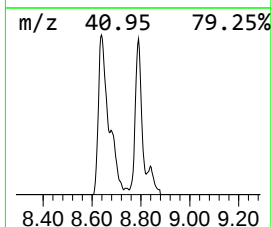
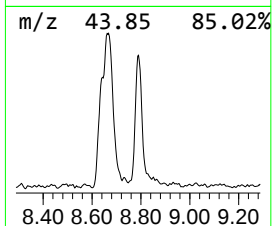
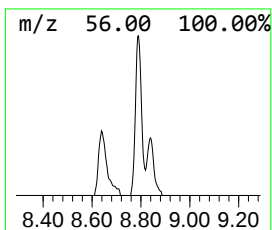
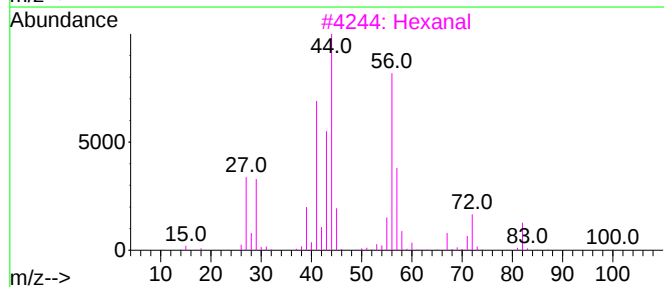
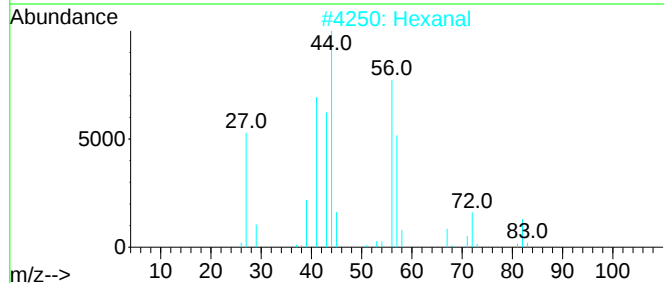
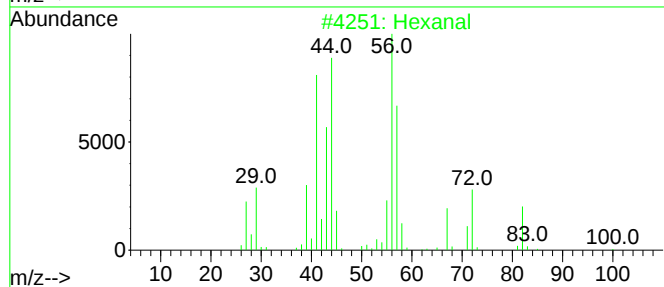
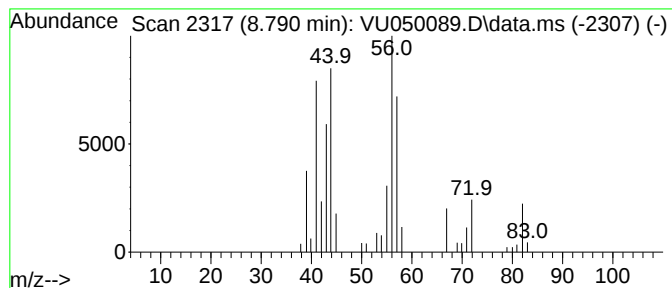
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.790	1.22 ug/L	53451	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	78
3	Hexanal			100	C6H12O	000066-25-1	78
4	Hexanal			100	C6H12O	000066-25-1	72
5	Hexanal			100	C6H12O	000066-25-1	64



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E53

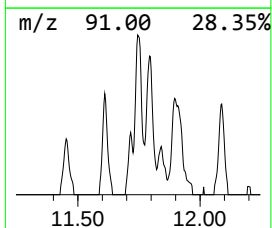
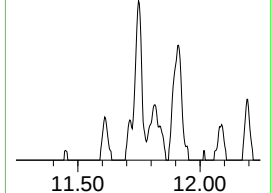
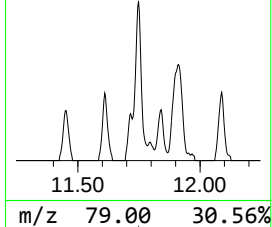
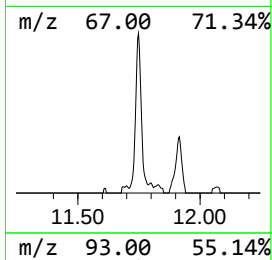
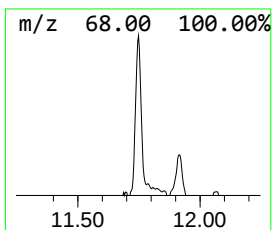
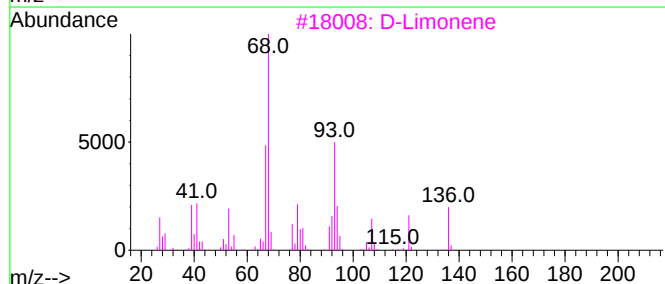
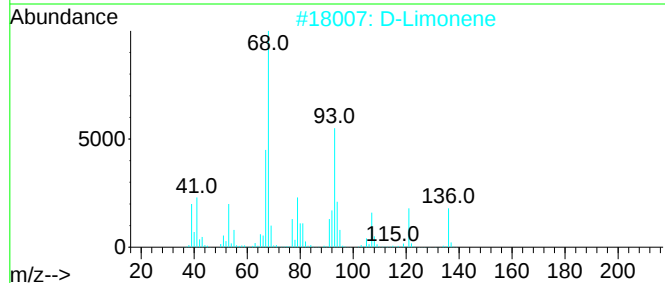
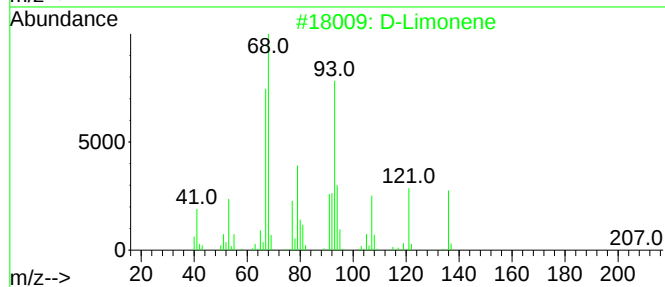
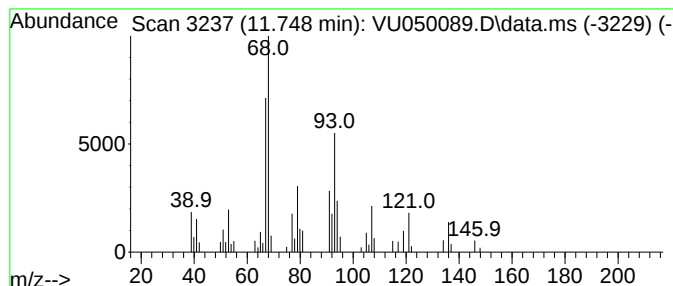
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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	61894	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene			136	C10H16	005989-27-5	98
2	D-Limonene			136	C10H16	005989-27-5	93
3	D-Limonene			136	C10H16	005989-27-5	93
4	D-Limonene			136	C10H16	005989-27-5	93
5	Limonene			136	C10H16	000138-86-3	93



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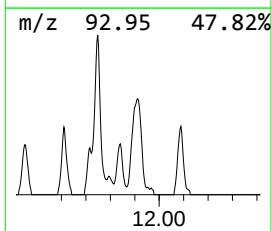
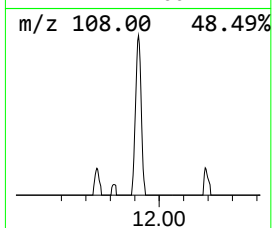
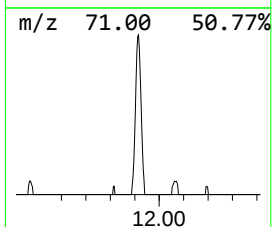
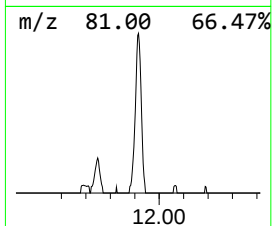
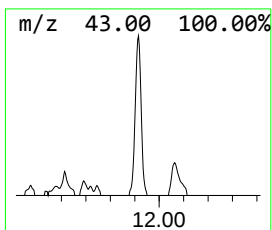
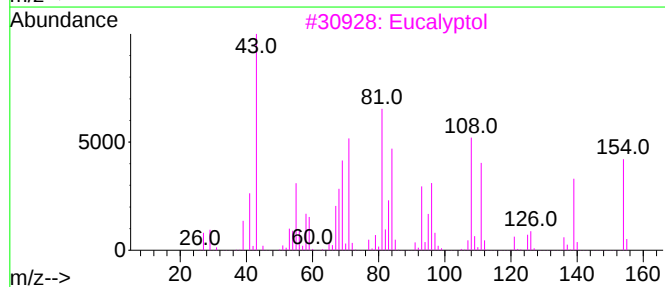
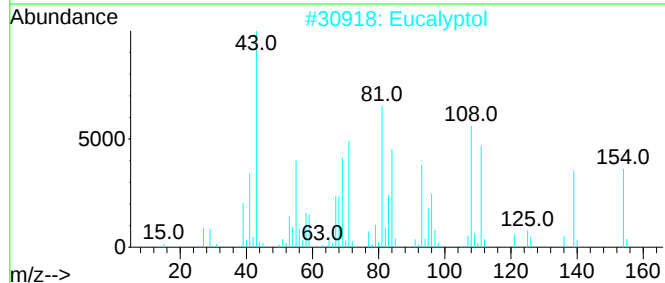
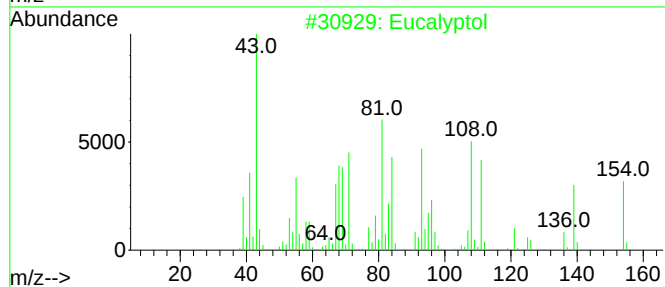
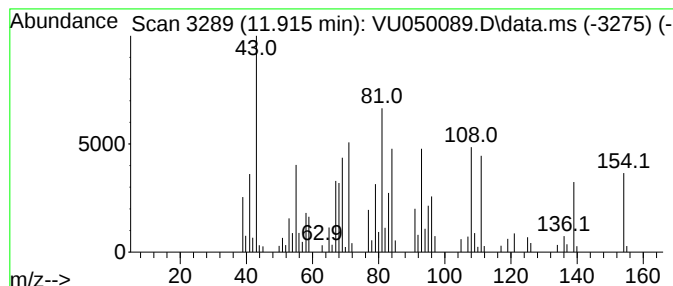
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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	1.81 ug/L	88122	1,4-Dichlorobenzene-d4	11.816

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	89
5	Trifluoroacetyl-.alpha.-terpineol			250	C12H17F3O2	1000058-17-6	87



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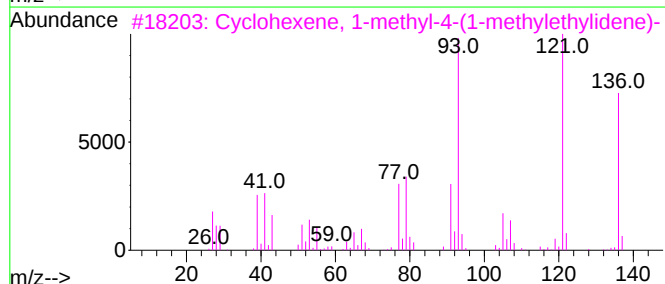
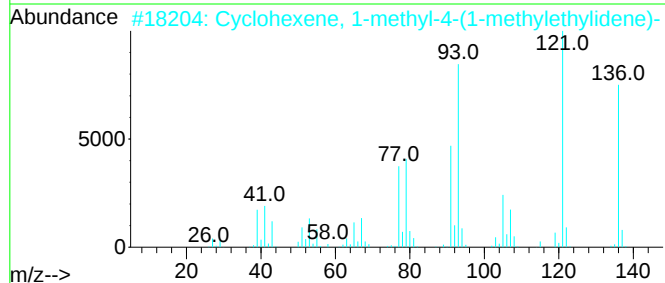
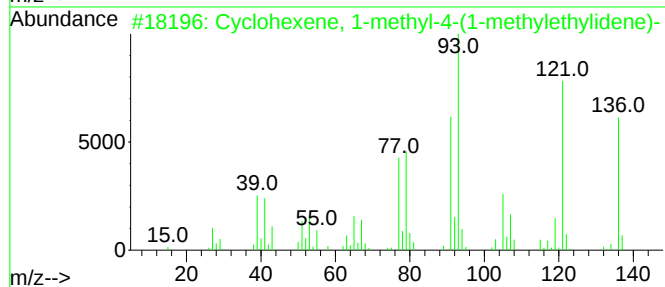
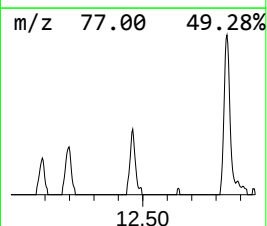
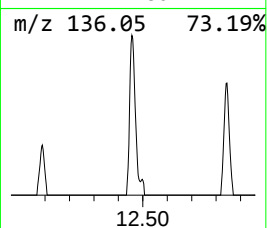
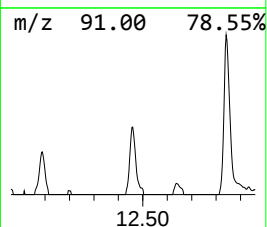
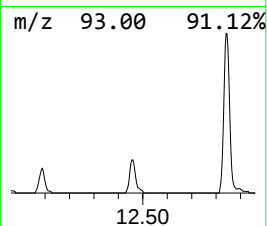
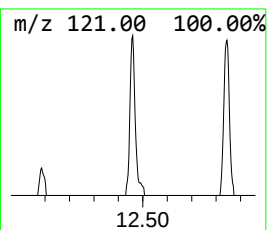
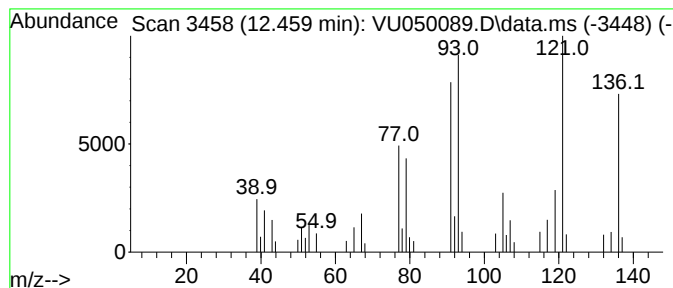
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.459	0.62 ug/L	29968	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	96
2			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	95
3			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	93
4			(+)-4-Carene	136	C10H16	029050-33-7	93
5			2-Carene	136	C10H16	000554-61-0	91



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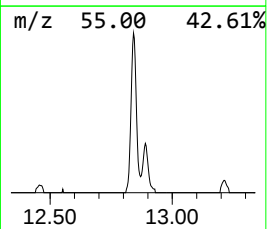
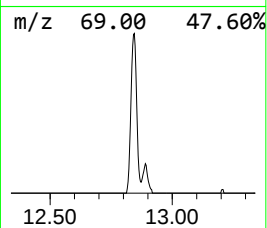
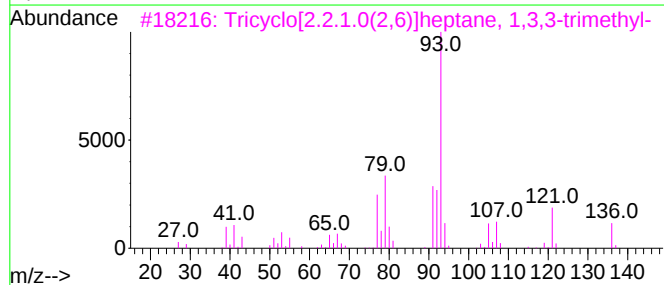
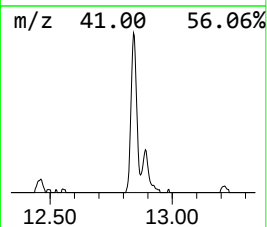
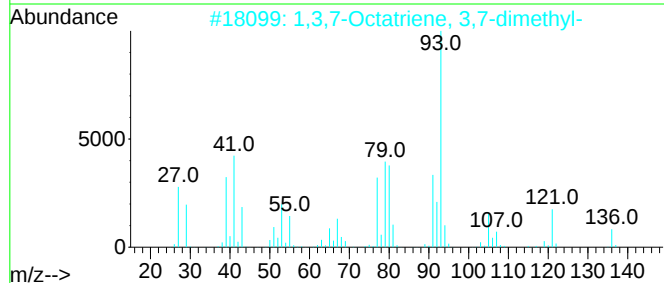
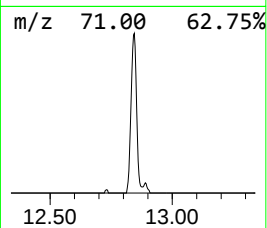
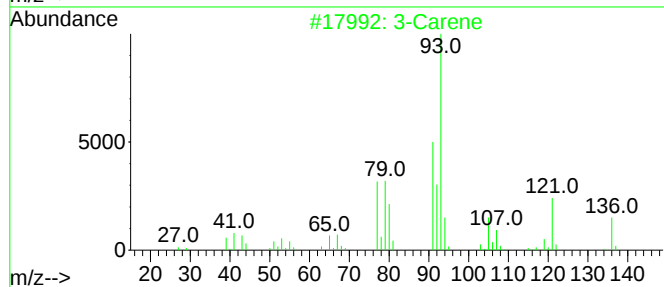
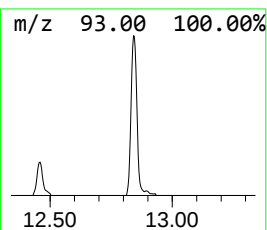
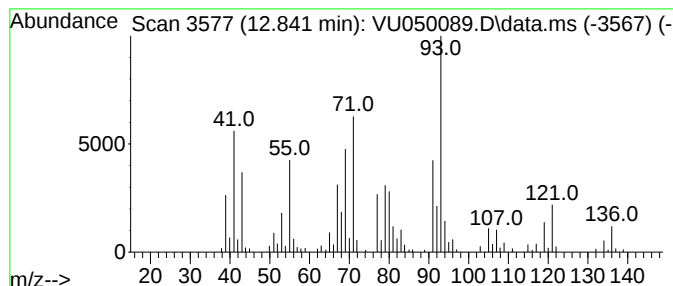
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 3-Carene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.841	2.96 ug/L	143811	1,4-Dichlorobenzene-d4	11.816

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	95
3			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	93
4			3-Carene	136	C10H16	013466-78-9	93
5			.beta.-Ocimene	136	C10H16	013877-91-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
Data File : VU050089.D
Acq On : 05 Aug 2022 11:38
Operator : SY/MD
Sample : N4022-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E53

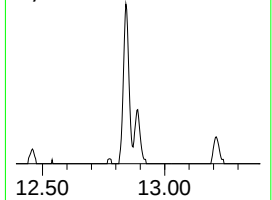
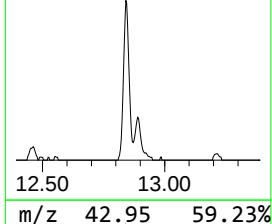
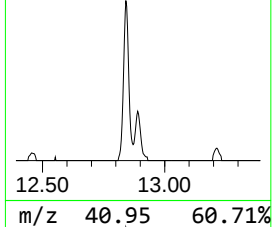
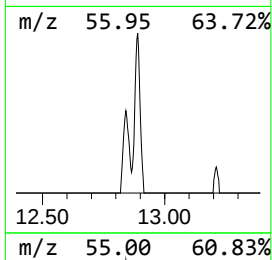
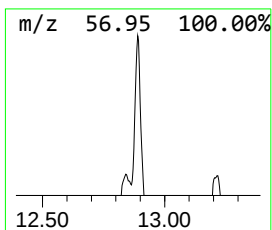
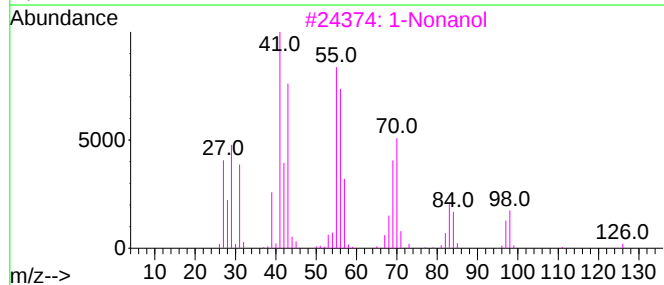
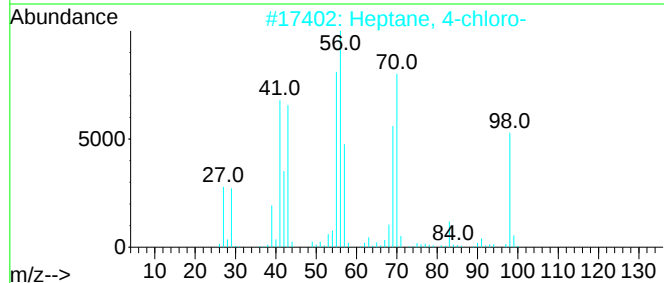
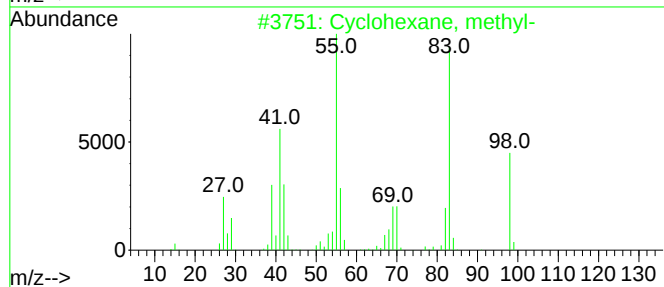
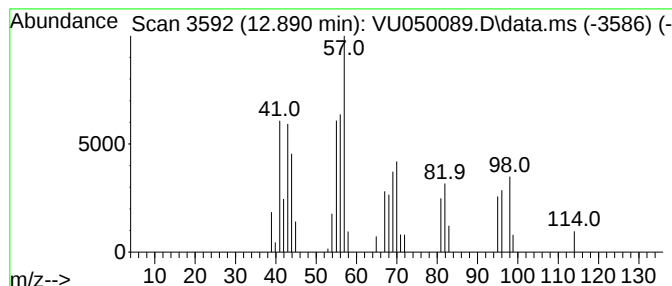
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 (DEL) Alkane: Cyclic12.890 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	0.62 ug/L	30257	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, methyl-	98	C7H14	000108-87-2	47
2			Heptane, 4-chloro-	134	C7H15Cl	000998-95-8	27
3			1-Nonanol	144	C9H20O	000143-08-8	27
4			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27
5			Cyanoacetic acid, heptyl ester	183	C10H17NO2	1000406-22-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
Data File : VU050089.D
Acq On : 05 Aug 2022 11:38
Operator : SY/MD
Sample : N4022-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E53

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	8.790	1.2	ug/L	53451	2	9.420	219239	5.0
D-Limonene	11.748	1.3	ug/L	61894	3	11.816	242890	5.0
Eucalyptol	11.915	1.8	ug/L	88122	3	11.816	242890	5.0
Cyclohexene, 1-...	12.459	0.6	ug/L	29968	3	11.816	242890	5.0
3-Carene	12.841	3.0	ug/L	143811	3	11.816	242890	5.0
(DEL) Alkane: C...	12.890	0.6	ug/L	30257	3	11.816	242890	5.0