

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
 Data File : VU050090.D
 Acq On : 05 Aug 2022 12:02
 Operator : SY/MD
 Sample : N4022-13
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5E55

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: VU050090.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	71	79	98	rVB	45103	52053	12.21%	1.373%
2	1.909	169	177	191	rBV	38341	48645	11.41%	1.283%
3	2.562	369	380	394	rVB	70087	110417	25.89%	2.913%
4	3.041	518	529	545	rVB	31213	57206	13.41%	1.509%
5	4.639	1012	1026	1071	rBV2	51326	174790	40.99%	4.611%
6	4.819	1074	1082	1098	rVB5	2587	6588	1.54%	0.174%
7	5.063	1139	1158	1176	rBV	68834	153014	35.88%	4.037%
8	5.722	1341	1363	1387	rBV2	137660	356627	83.63%	9.408%
9	6.250	1512	1527	1545	rBV	105289	197680	46.35%	5.215%
10	6.690	1650	1664	1682	rBV	87928	171798	40.28%	4.532%
11	7.565	1923	1936	1956	rBV	41197	74081	17.37%	1.954%
12	7.899	2025	2040	2055	rBV	157655	275964	64.71%	7.280%
13	7.970	2056	2062	2072	rVB	3703	5861	1.37%	0.155%
14	8.182	2117	2128	2145	rBV2	25337	44183	10.36%	1.166%
15	8.639	2252	2270	2307	rBV3	176299	426459	100.00%	11.250%
16	8.790	2307	2317	2326	rVV2	30670	53655	12.58%	1.415%
17	8.838	2326	2332	2347	rVB2	8341	14178	3.32%	0.374%
18	9.417	2499	2512	2528	rBV	148412	247973	58.15%	6.542%
19	10.082	2710	2719	2739	rBV2	12094	22220	5.21%	0.586%
20	10.221	2752	2762	2778	rBV3	5608	9939	2.33%	0.262%
21	10.758	2918	2929	2944	rBV	75729	121049	28.38%	3.193%
22	11.163	3046	3055	3066	rBV4	9059	14828	3.48%	0.391%
23	11.378	3114	3122	3131	rVB3	3752	5458	1.28%	0.144%
24	11.449	3133	3144	3148	rBV2	5632	8512	2.00%	0.225%
25	11.610	3186	3194	3208	rVB3	16695	25789	6.05%	0.680%
26	11.693	3211	3220	3221	rBV4	4321	4488	1.05%	0.118%
27	11.745	3222	3236	3244	rVV	44645	80750	18.93%	2.130%
28	11.812	3244	3257	3274	rVV2	148407	279841	65.62%	7.382%
29	11.912	3274	3288	3302	rVB4	51771	98994	23.21%	2.612%
30	12.063	3322	3335	3340	rBV2	17685	30802	7.22%	0.813%
31	12.192	3363	3375	3389	rBV	153554	243815	57.17%	6.432%
32	12.455	3448	3457	3474	rBV3	23830	38090	8.93%	1.005%
33	12.642	3508	3515	3527	rVB3	3419	4913	1.15%	0.130%
34	12.841	3564	3577	3586	rBV	124822	196632	46.11%	5.187%
35	12.886	3586	3591	3609	rVB3	21440	35171	8.25%	0.928%
36	13.738	3843	3856	3869	rBV3	15085	24250	5.69%	0.640%

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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	13.835	3877	3886	3897	rBV2	14493	22084	5.18%	0.583%
38	14.034	3937	3948	3960	rBV2	32977	51889	12.17%	1.369%

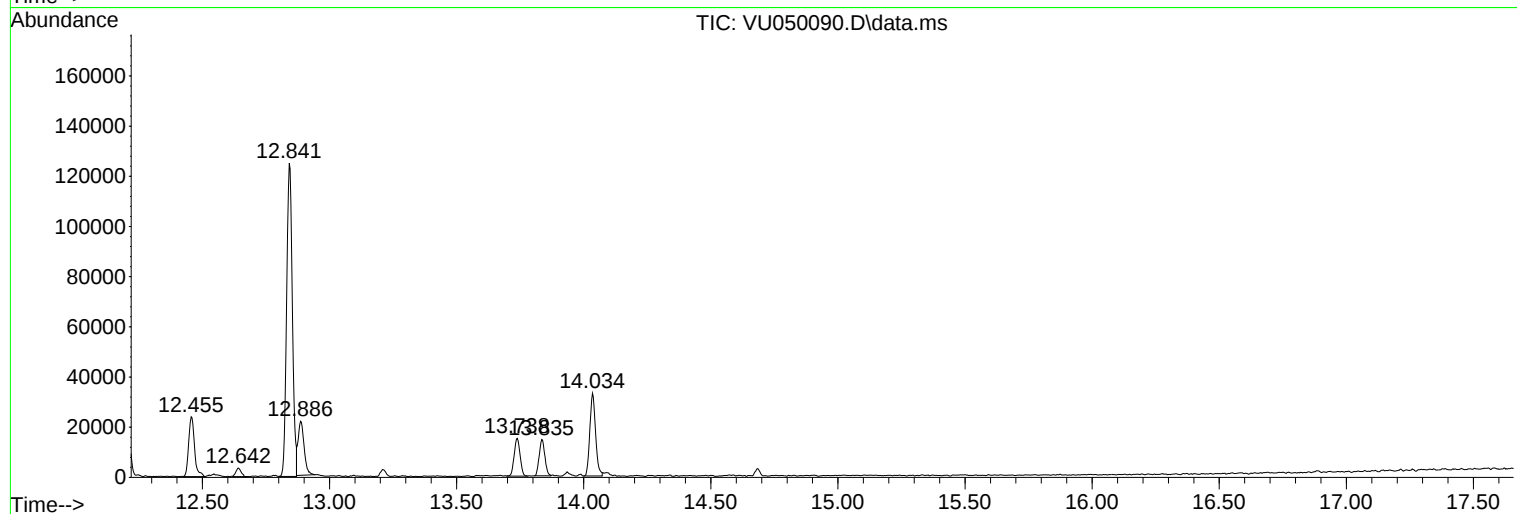
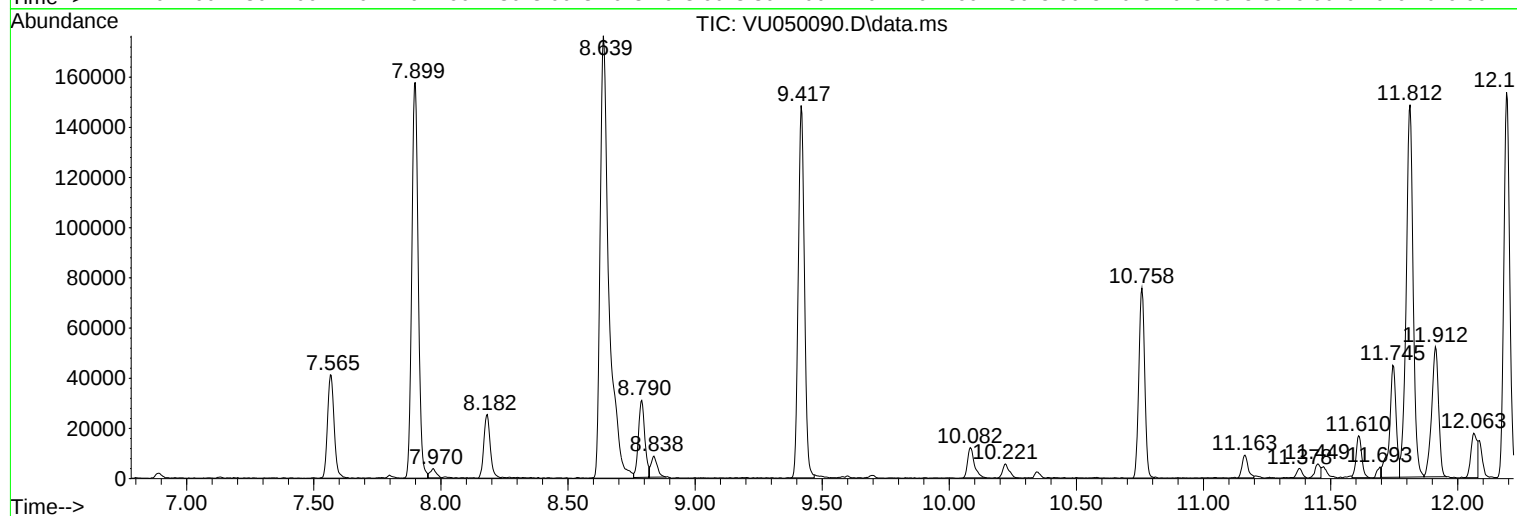
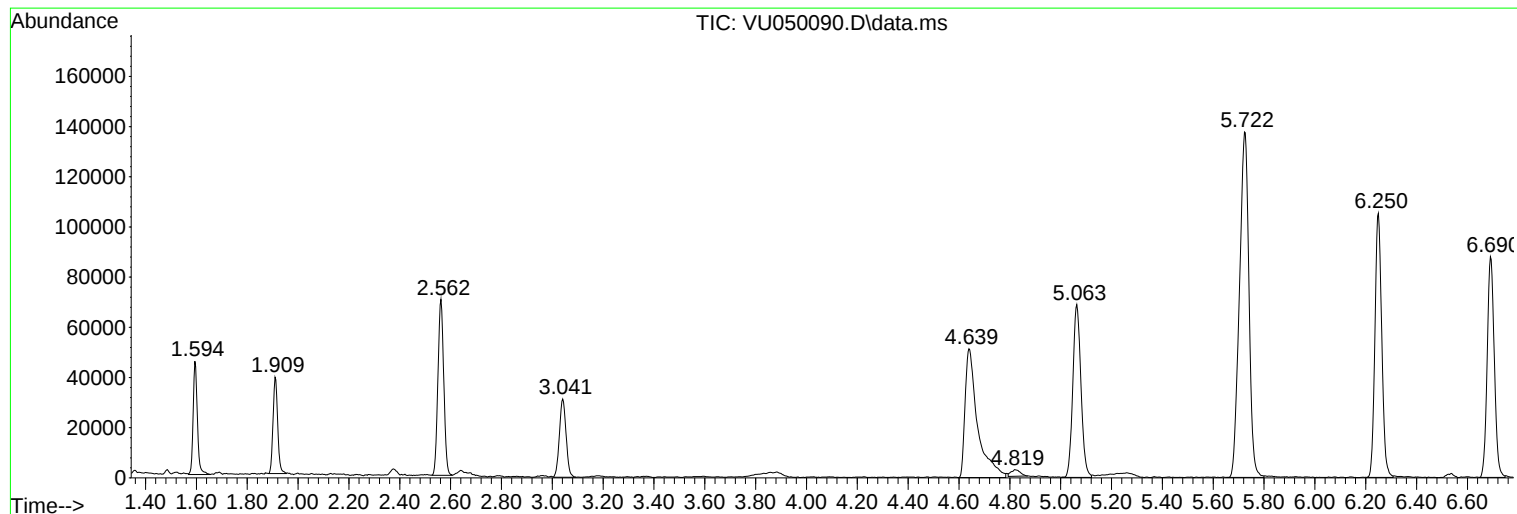
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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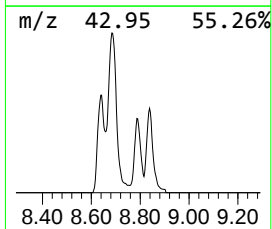
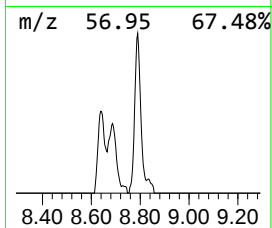
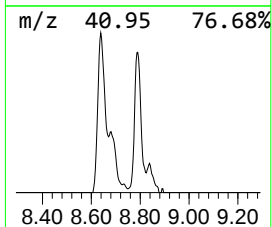
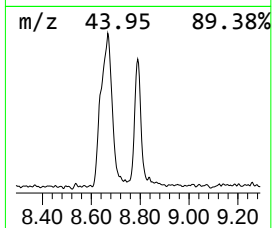
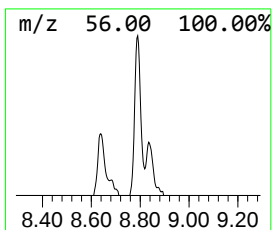
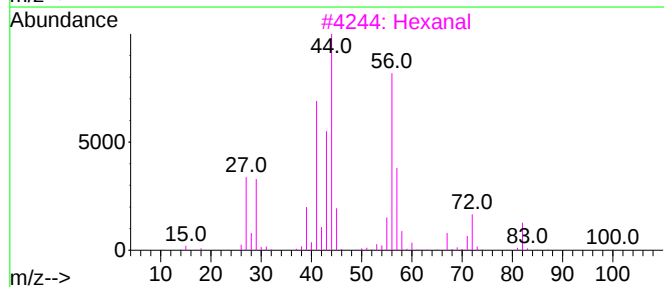
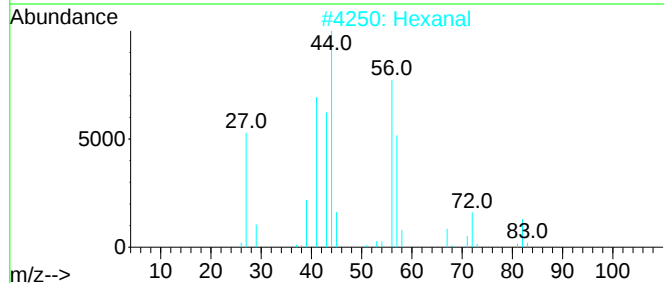
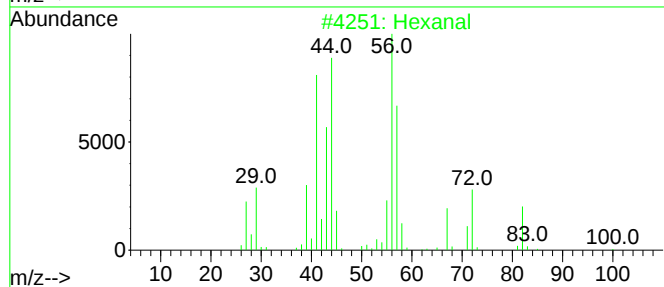
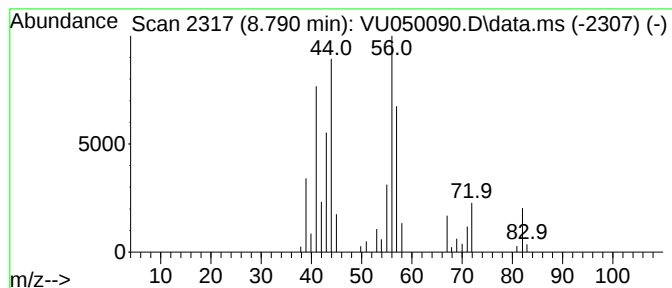
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
8.790	1.08 ug/L	53655	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	86
2	Hexanal			100	C6H12O	000066-25-1	80
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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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E55

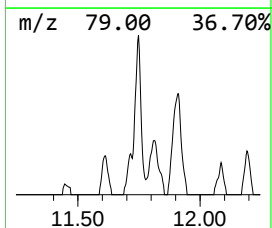
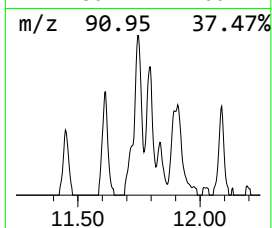
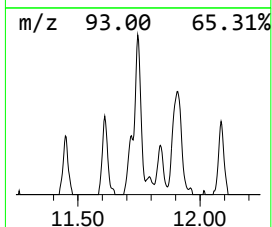
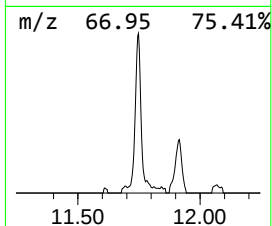
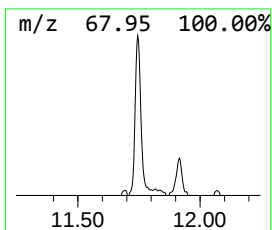
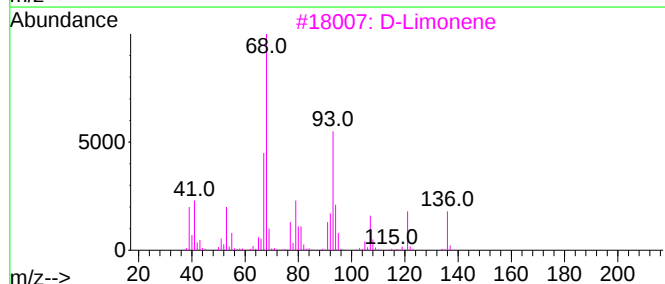
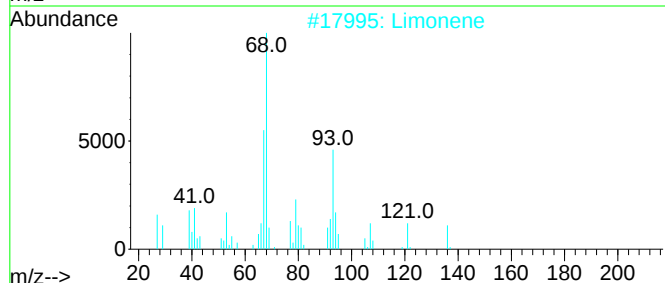
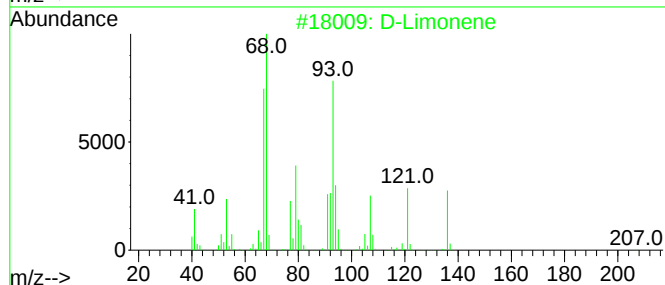
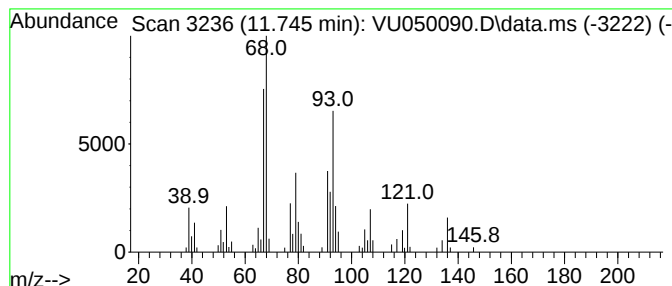
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
11.745	1.44 ug/L	80750	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			D-Limonene	136	C10H16	005989-27-5	96
2			Limonene	136	C10H16	000138-86-3	81
3			D-Limonene	136	C10H16	005989-27-5	81
4			Cyclohexene, 4-ethenyl-1,4-dimet...	136	C10H16	001743-61-9	72
5			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	005989-54-8	70



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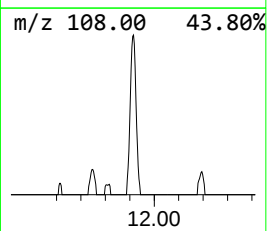
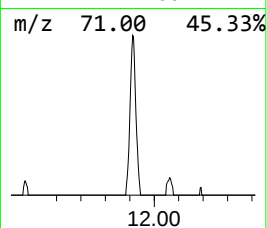
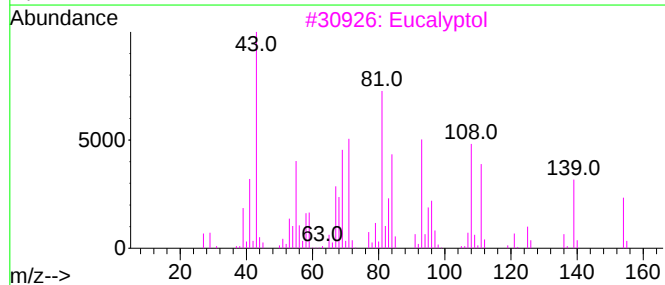
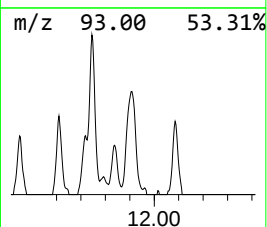
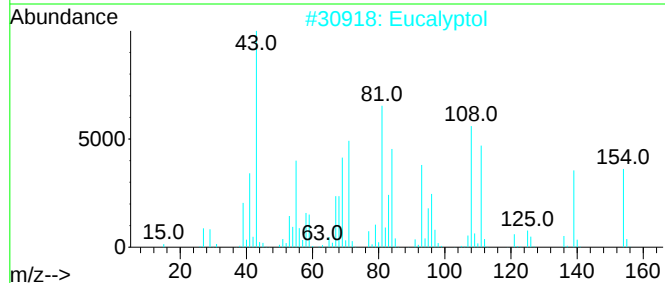
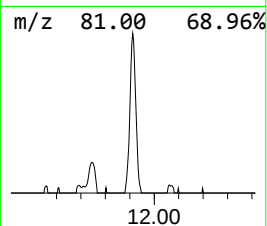
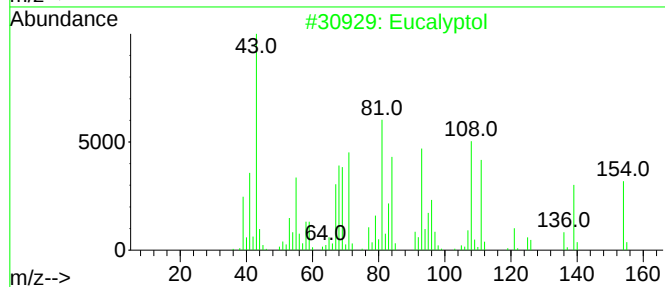
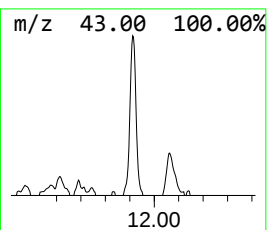
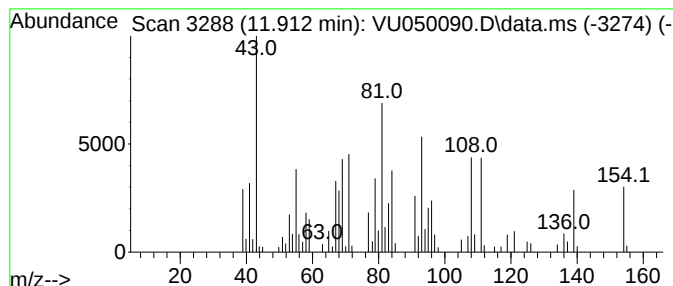
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
11.912	1.77 ug/L	98994	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	96
3	Eucalyptol			154	C10H18O	000470-82-6	95
4	Eucalyptol			154	C10H18O	000470-82-6	94
5	Eucalyptol			154	C10H18O	000470-82-6	91



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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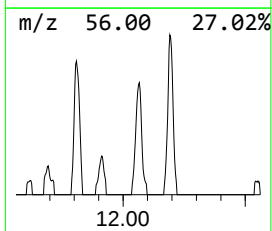
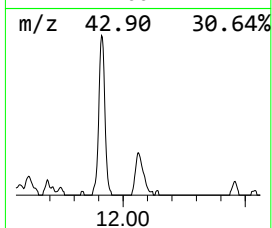
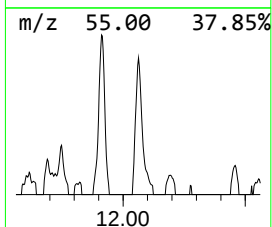
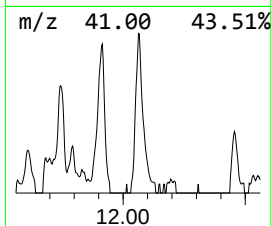
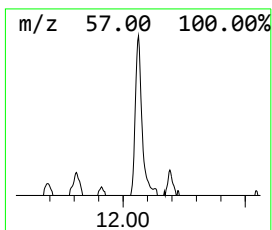
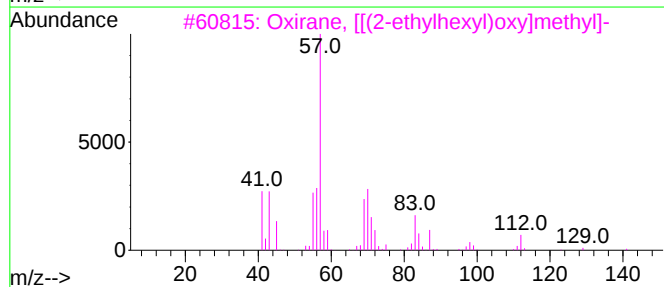
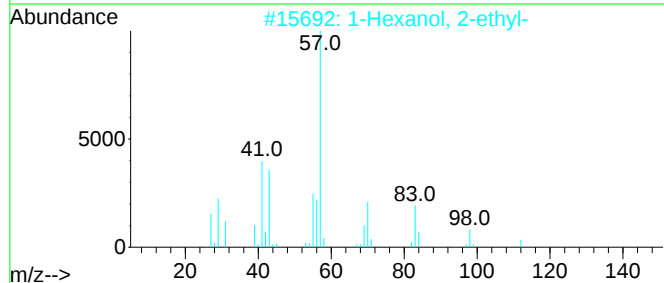
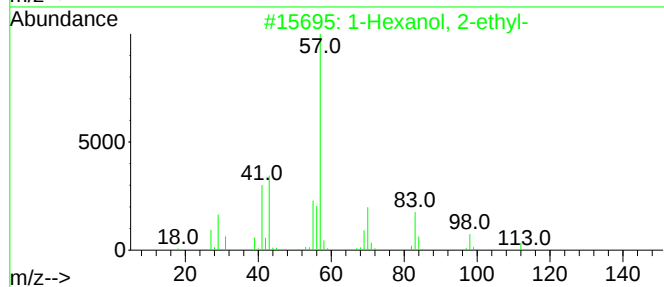
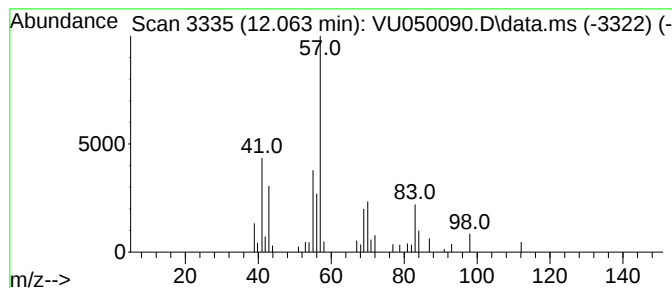
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	0.55 ug/L	30802	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3			Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	72
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



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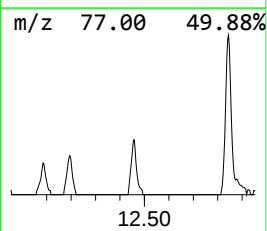
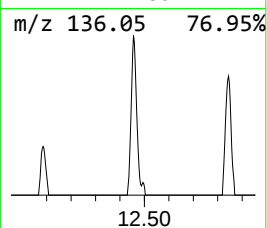
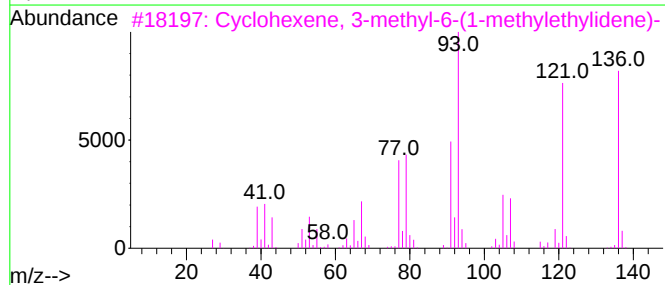
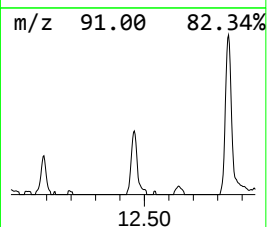
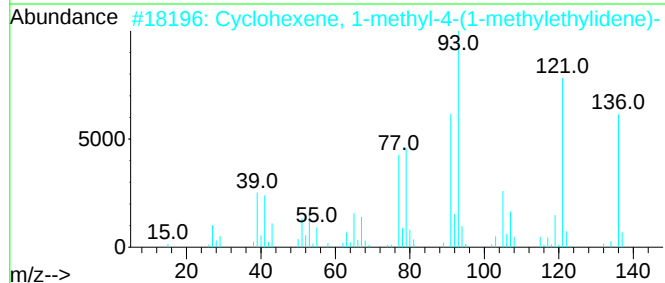
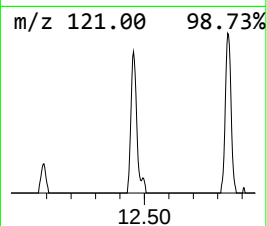
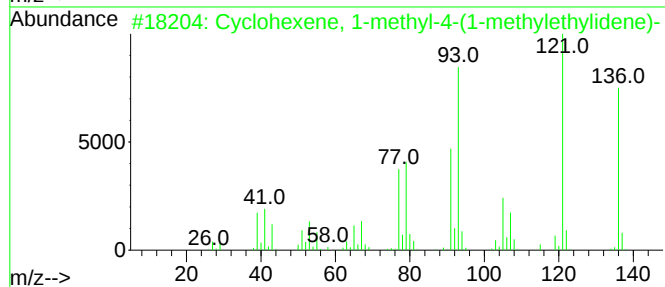
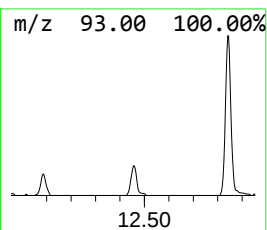
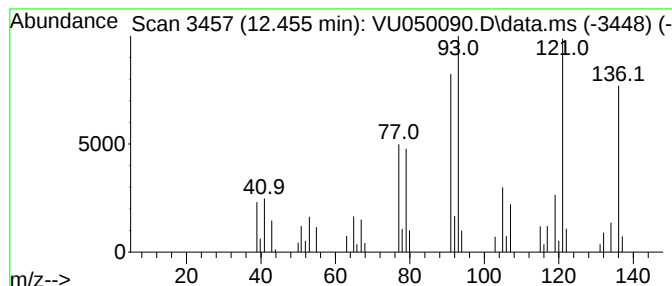
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.455	0.68 ug/L	38090	1,4-Dichlorobenzene-d4	11.812

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	96
3			Cyclohexene, 3-methyl-6-(1-methy...	136	C10H16	000586-63-0	94
4			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	93
5			2-Carene	136	C10H16	000554-61-0	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
Data File : VU050090.D
Acq On : 05 Aug 2022 12:02
Operator : SY/MD
Sample : N4022-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

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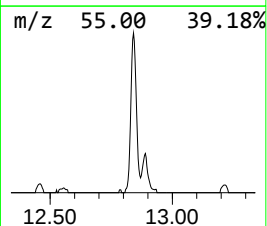
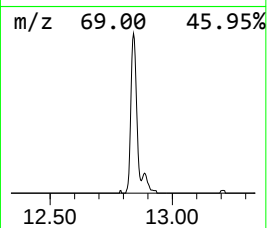
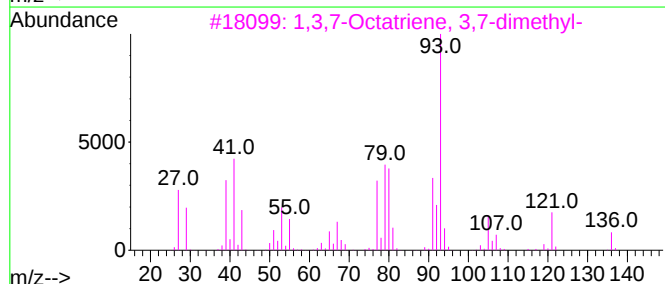
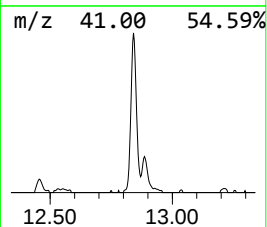
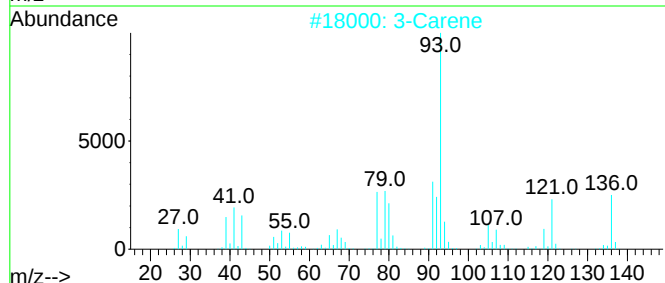
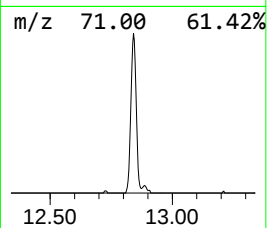
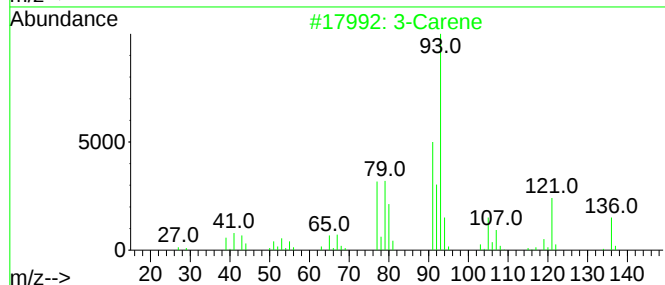
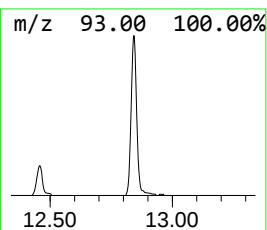
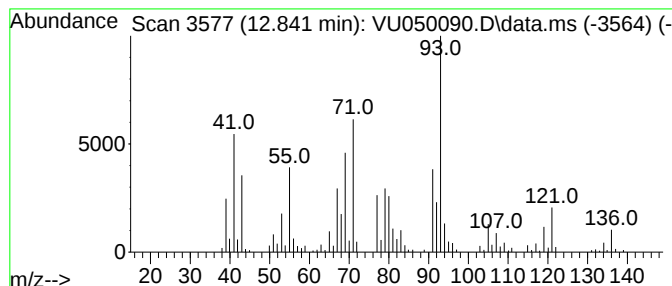
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 3-Carene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.841	3.51 ug/L	196632	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			3-Carene	136	C10H16	013466-78-9	93
3			1,3,7-Octatriene, 3,7-dimethyl-	136	C10H16	000502-99-8	92
4			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	91
5			3-Carene	136	C10H16	013466-78-9	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
Data File : VU050090.D
Acq On : 05 Aug 2022 12:02
Operator : SY/MD
Sample : N4022-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E55

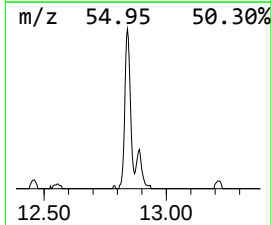
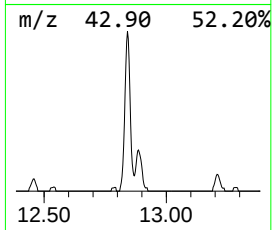
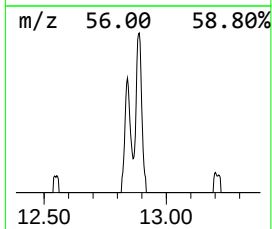
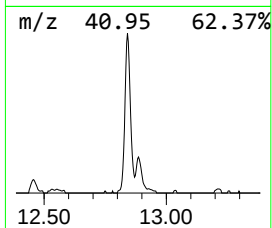
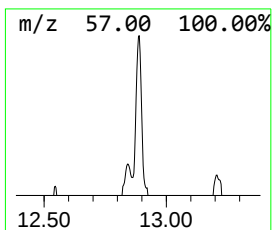
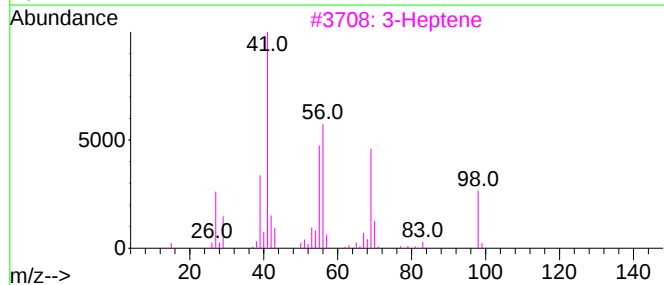
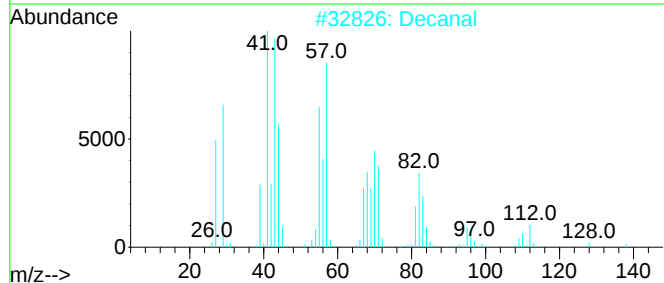
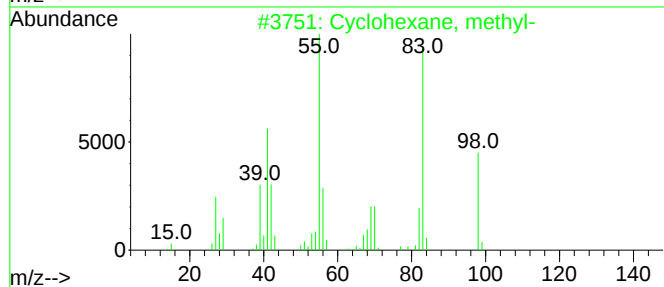
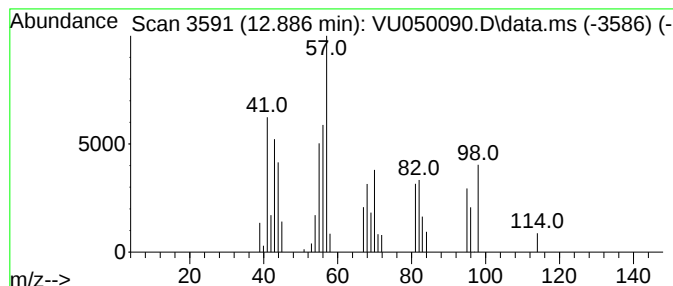
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 (DEL) Alkane: Cyclic12.886 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	0.63 ug/L	35171	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, methyl-	98	C7H14	000108-87-2	49
2			Decanal	156	C10H20O	000112-31-2	37
3			3-Heptene	98	C7H14	000592-78-9	27
4			3-Heptene, (E)-	98	C7H14	014686-14-7	22
5			Oxirane, decyl-	184	C12H24O	002855-19-8	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
Data File : VU050090.D
Acq On : 05 Aug 2022 12:02
Operator : SY/MD
Sample : N4022-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E55

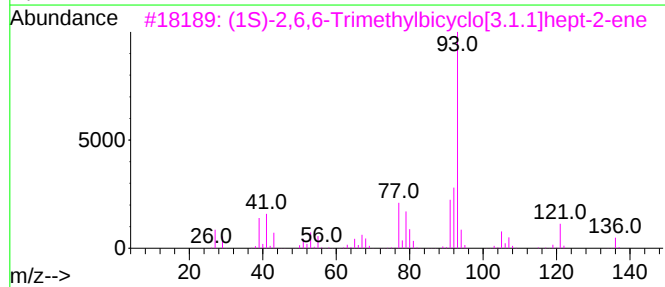
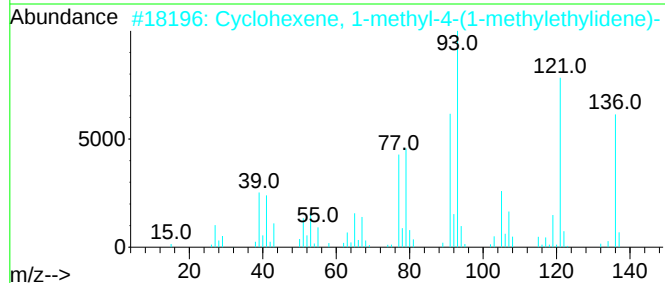
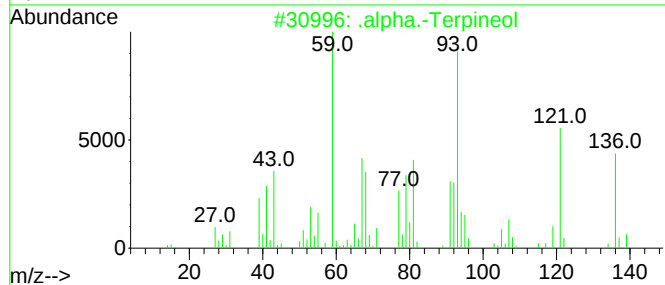
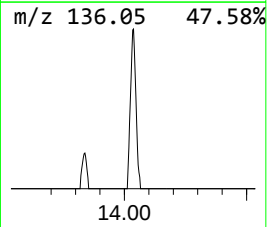
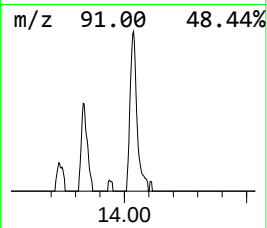
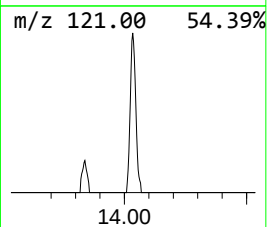
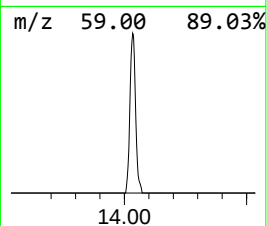
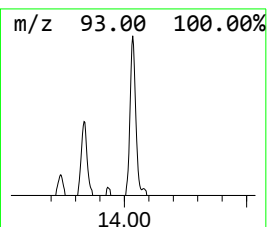
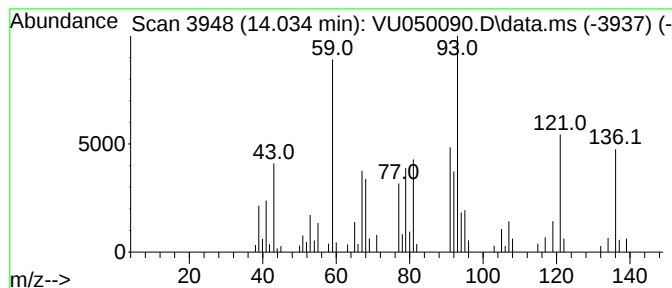
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 .alpha.-Terpineol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.034	0.93 ug/L	51889	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			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	83
3			(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	64
4			3-Carene	136	C10H16	013466-78-9	64
5			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080522\
Data File : VU050090.D
Acq On : 05 Aug 2022 12:02
Operator : SY/MD
Sample : N4022-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5E55

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	1.1	ug/L	53655	2	9.417	247973	5.0
D-Limonene	11.745	1.4	ug/L	80750	3	11.812	279841	5.0
Eucalyptol	11.912	1.8	ug/L	98994	3	11.812	279841	5.0
1-Hexanol, 2-et...	12.063	0.6	ug/L	30802	3	11.812	279841	5.0
Cyclohexene, 1-...	12.455	0.7	ug/L	38090	3	11.812	279841	5.0
3-Carene	12.841	3.5	ug/L	196632	3	11.812	279841	5.0
(DEL) Alkane: C...	12.886	0.6	ug/L	35171	3	11.812	279841	5.0
.alpha.-Terpineol	14.034	0.9	ug/L	51889	3	11.812	279841	5.0