

Data Path : Z:\voasrv\HPCHEM1\MSVOA_L\Data\VL040725\
 Data File : VL042247.D
 Acq On : 07 Apr 2025 23:41
 Operator : SY/MD
 Sample : Q1725-06 4X
 Misc : 400mL/MSVOA_L
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_L
 ClientSampleId :
 SSSG-B10-3-03312025

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 3

Min Area: 3 % of largest Peak

Start Thrs: 0.001

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 0

Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M

Title : AIR ANALYSIS BY METHOD TO-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

Signal : TIC: VL042247.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.434	412	416	417	rBV	4572470	2968303	77.19%	10.875%
2	1.441	417	418	423	rVB2	4313247	2274854	59.16%	8.335%
3	1.496	431	435	442	rVB2	137903	71295	1.85%	0.261%
4	1.567	452	457	461	rBV	145674	88784	2.31%	0.325%
5	1.732	503	508	518	rBV	3297358	2194029	57.06%	8.039%
6	1.845	538	543	552	rBV	2505629	1701485	44.25%	6.234%
7	1.897	554	559	572	rVB	4384027	3299416	85.80%	12.089%
8	2.072	609	613	621	rVB	126474	96500	2.51%	0.354%
9	2.573	761	768	779	rBV	298033	286473	7.45%	1.050%
10	2.803	831	839	846	rBV	703471	737338	19.17%	2.701%
11	2.845	846	852	857	rBV3	58253	82458	2.14%	0.302%
12	3.985	1189	1204	1217	rBV	877806	1336388	34.75%	4.896%
13	8.247	2512	2521	2532	rBV3	69195	115249	3.00%	0.422%
14	8.904	2711	2724	2735	rBV	1130973	1555835	40.46%	5.700%
15	9.173	2794	2807	2831	rBV	2502936	3429931	89.20%	12.567%
16	10.396	3171	3185	3196	rBV	1496947	1730228	45.00%	6.339%
17	11.558	3534	3544	3553	rBV5	30551	51520	1.34%	0.189%
18	12.060	3686	3699	3722	rBV	3787176	3845359	100.00%	14.089%
19	12.442	3806	3817	3827	rBV7	132226	193331	5.03%	0.708%
20	12.720	3897	3903	3918	rVB2	150377	163894	4.26%	0.600%
21	13.400	4104	4113	4122	rBV	1131169	1071024	27.85%	3.924%

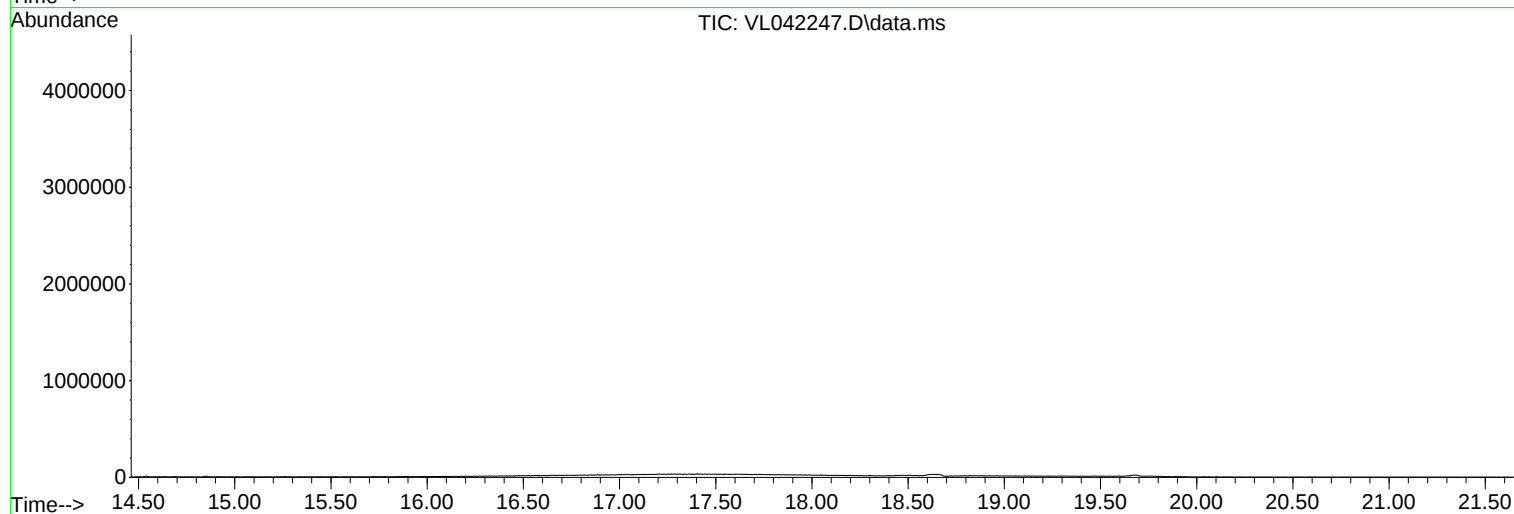
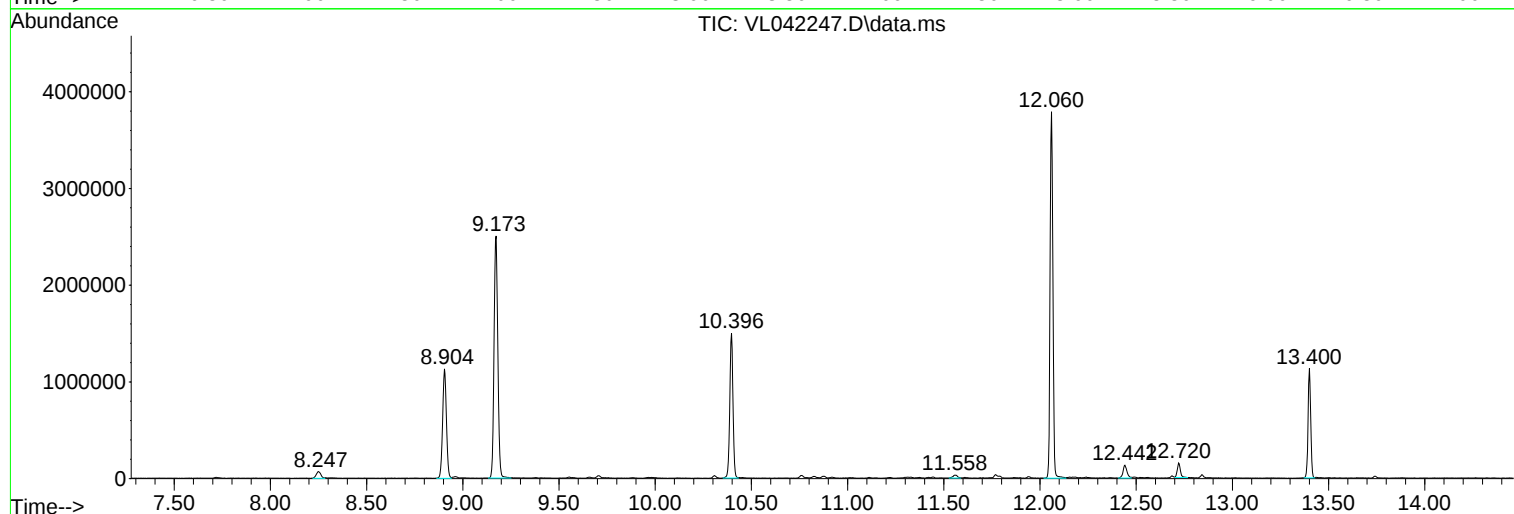
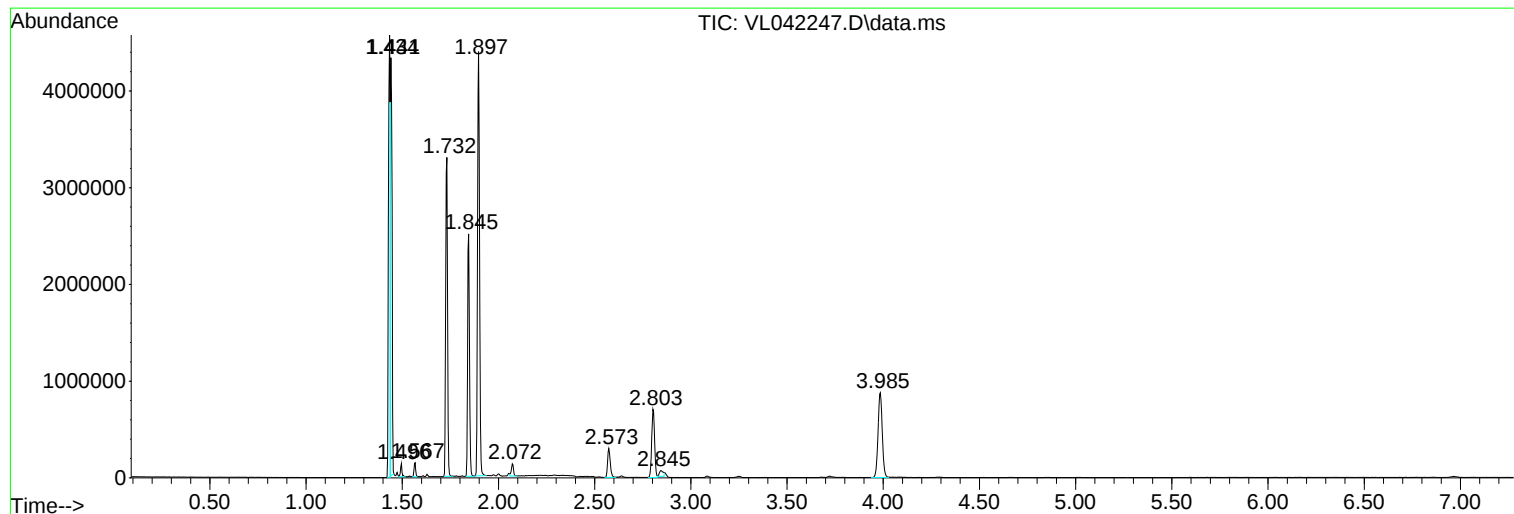
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_L
ClientSampleId :
SSSG-B10-3-03312025

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD TO-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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



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Instrument :
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ClientSampleId :
SSSG-B10-3-03312025

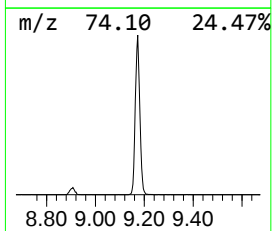
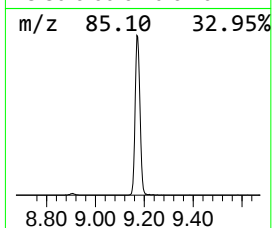
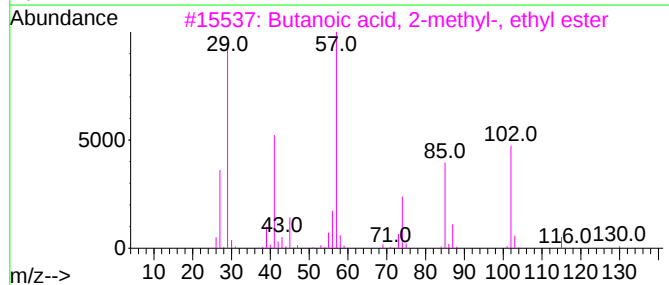
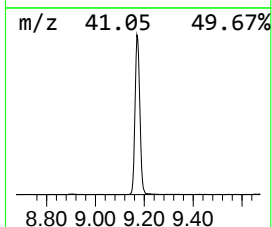
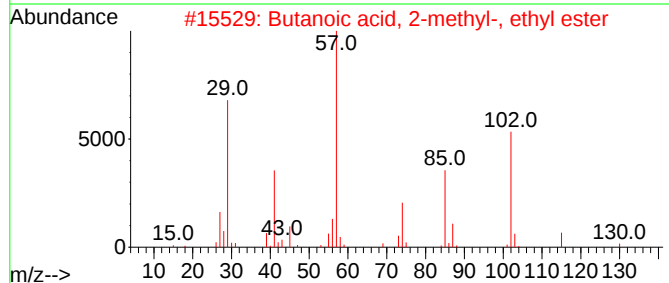
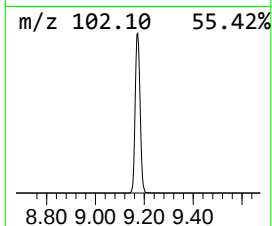
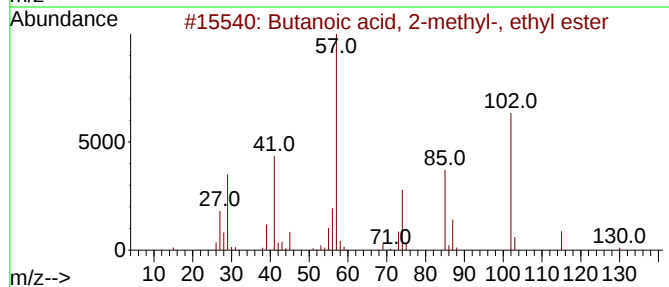
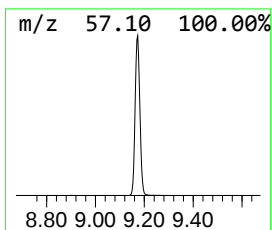
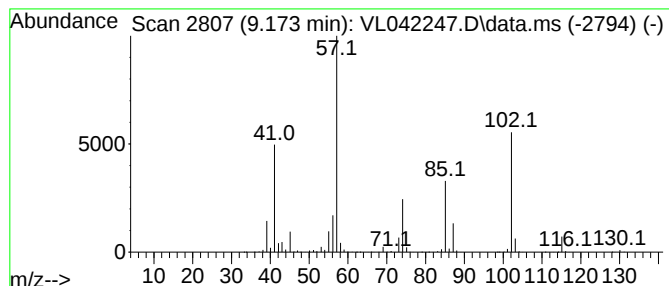
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 3 Butanoic acid, 2-methyl-, e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.173	22.05 ppbv	3429930	Chlorobenzene-d5	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	93
2			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	91
3			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	90
4			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	83
5			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	74



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Instrument :
MSVOA_L
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SSSG-B10-3-03312025

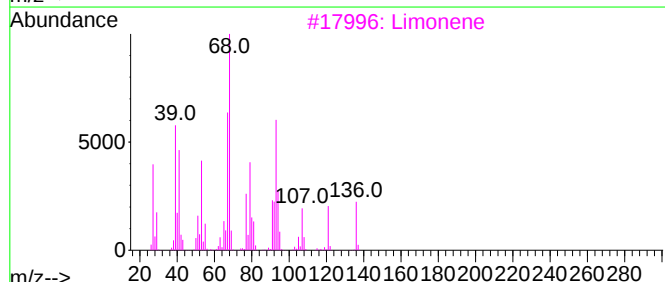
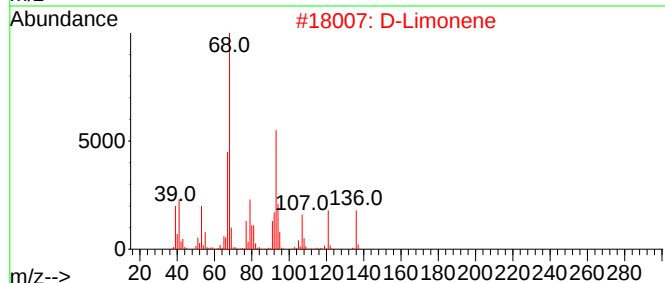
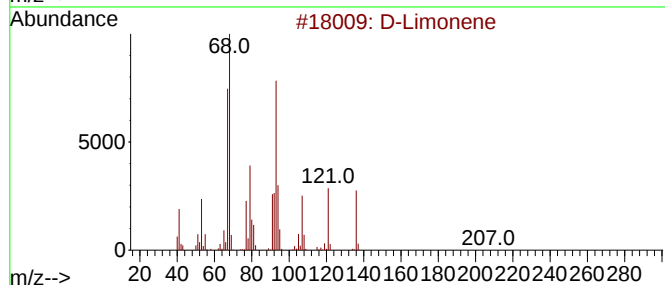
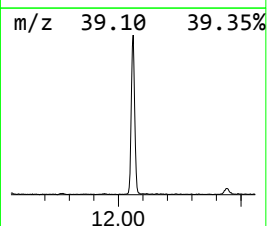
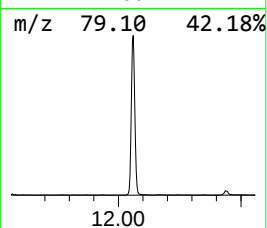
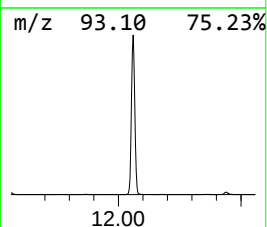
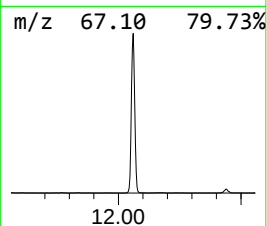
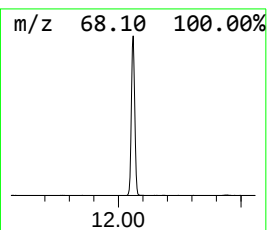
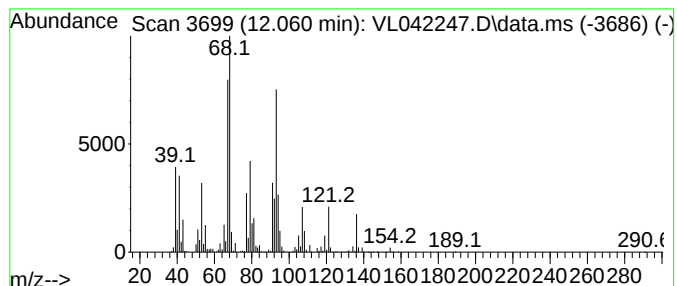
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD TO-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 4 D-Limonene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	24.72 ppbv	3845360	Chlorobenzene-d5	8.904

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	94
3			Limonene	136	C10H16	000138-86-3	94
4			D-Limonene	136	C10H16	005989-27-5	93
5			D-Limonene	136	C10H16	005989-27-5	93



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Misc : 400mL/MSVOA_L
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_L
ClientSampleId :
SSSG-B10-3-03312025

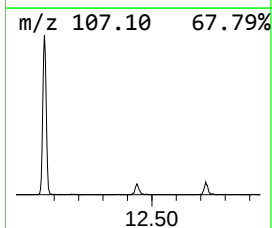
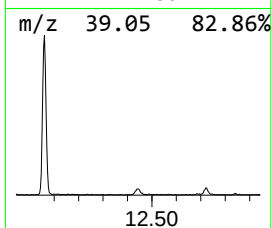
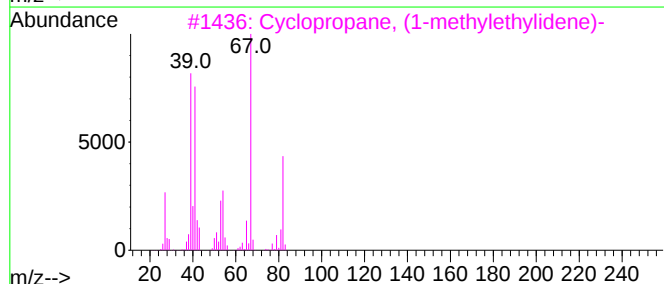
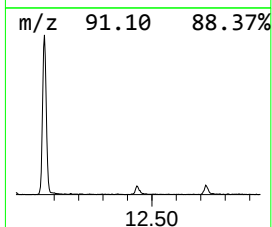
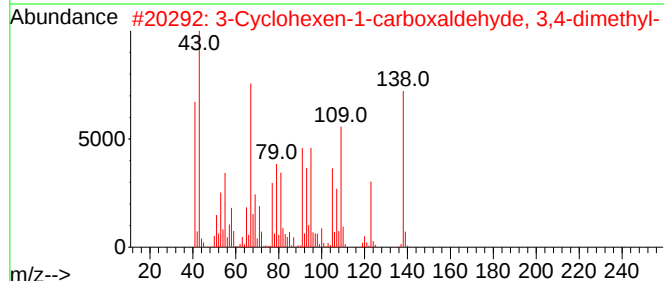
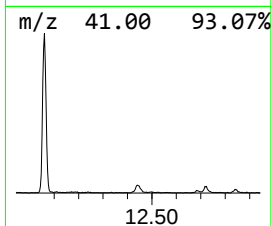
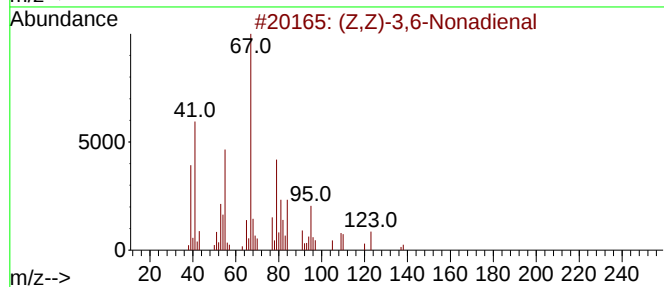
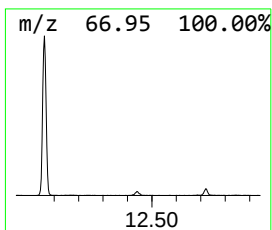
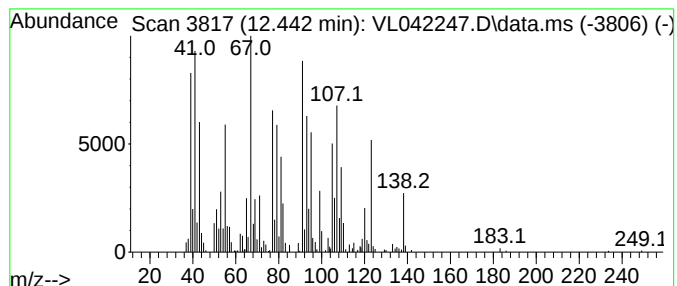
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 5 (Z,Z)-3,6-Nonadienal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.442	1.24 ppbv	193331	Chlorobenzene-d5	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(Z,Z)-3,6-Nonadienal	138	C9H14O	021944-83-2	80
2			3-Cyclohexen-1-carboxaldehyde, 3...	138	C9H14O	1000131-99-4	55
3			Cyclopropane, (1-methylethylidene)-	82	C6H10	004741-86-0	53
4			2,4-Dimethylcyclohex-3-ene-1-car...	138	C9H14O	068039-49-6	49
5			4-Methyl-2-pentyne	82	C6H10	021020-27-9	49



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Misc : 400mL/MSVOA_L
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_L
ClientSampleId :
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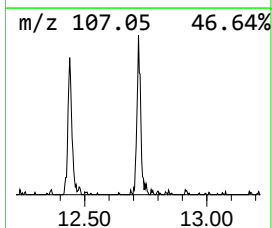
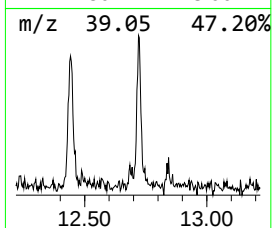
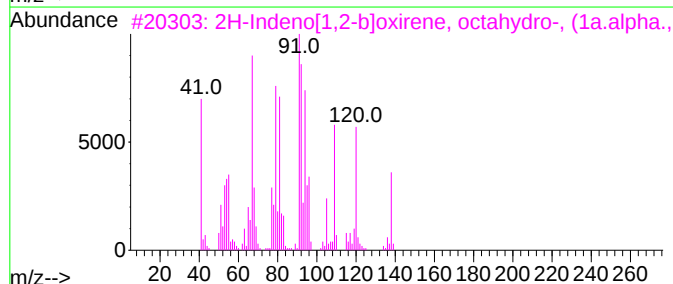
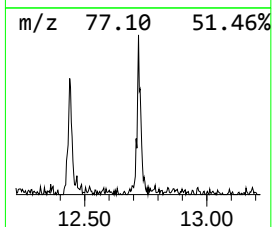
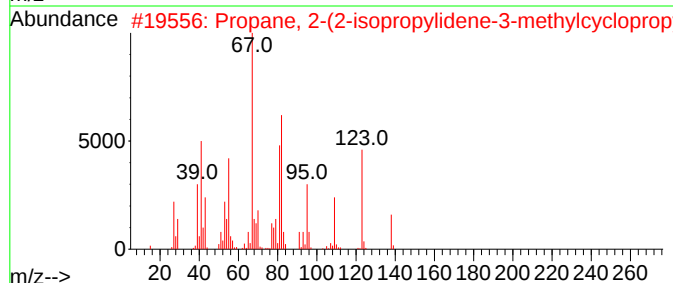
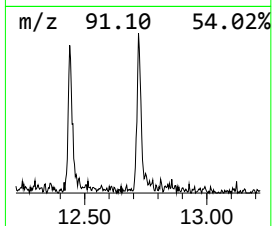
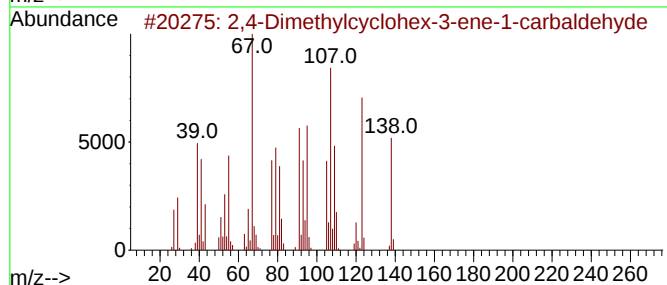
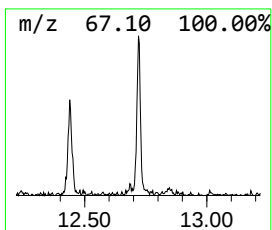
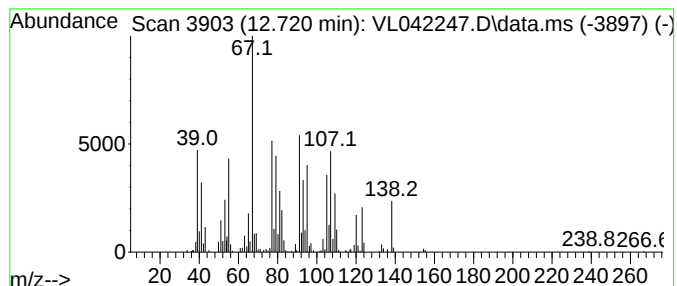
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 6 unknown12.720 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.720	1.05 ppbv	163894	Chlorobenzene-d5	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dimethylcyclohex-3-ene-1-car...	138	C9H14O	068039-49-6	46
2			Propane, 2-(2-isopropylidene-3-m...	138	C10H18	024524-51-4	46
3			2H-Indeno[1,2-b]oxirene, octahyd...	138	C9H14O	055402-31-8	38
4			3-Octyne	110	C8H14	015232-76-5	30
5			1,3-Hexadiene, 3-ethyl-2,5-dimet...	138	C10H18	062338-07-2	18



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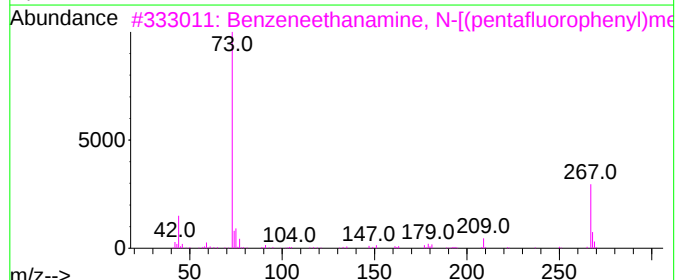
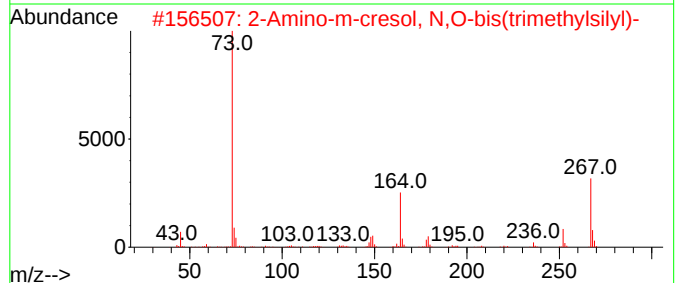
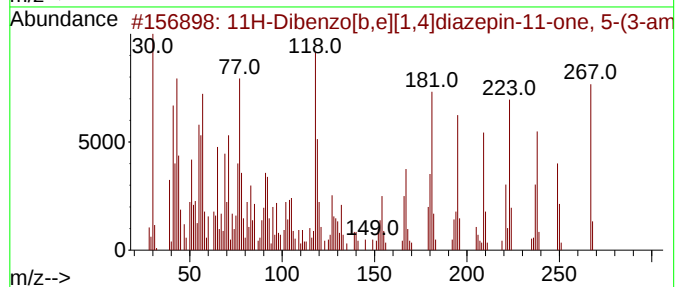
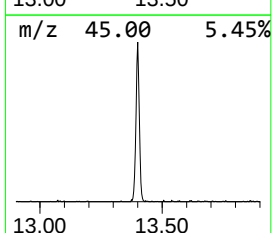
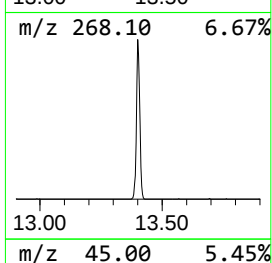
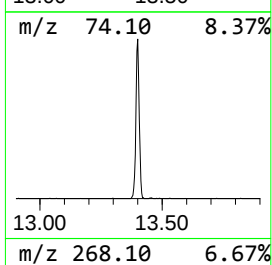
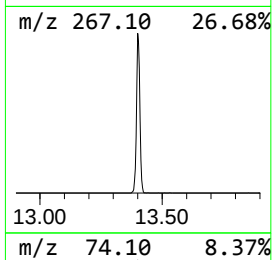
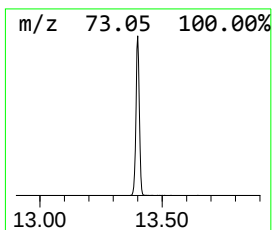
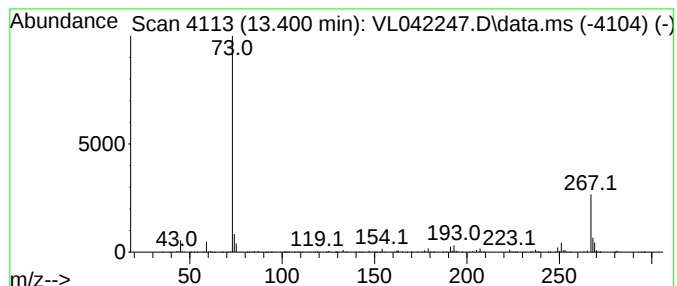
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 7 11H-Dibenzo[b,e][1,4]diazep... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.400	6.88 ppbv	1071020	Chlorobenzene-d5	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	94
2			2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	59
3			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	50
4			2-[(Trimethylsilyl)oxy]-2-{4-[(t...	297	C14H27NO2Si2	1000473-27-9	40
5			Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	40



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD TO-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, ...	9.173	22.1	ppbv	3429930	3	8.904	1555840	10.0
D-Limonene	12.060	24.7	ppbv	3845360	3	8.904	1555840	10.0
(Z,Z)-3,6-Nonad...	12.442	1.2	ppbv	193331	3	8.904	1555840	10.0
unknown12.720	12.720	1.1	ppbv	163894	3	8.904	1555840	10.0
11H-Dibenzo[b,e...	13.400	6.9	ppbv	1071020	3	8.904	1555840	10.0