

Data Path : Z:\voasrv\HPCHEM1\MSVOA_L\Data\VL040825\
 Data File : VL042256.D
 Acq On : 08 Apr 2025 10:55
 Operator : SY/MD
 Sample : Q1725-03
 Misc : 400mL/MSVOA_L
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_L
 ClientSampleId :
 SSSG-DUP-2-04012025

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: VL042256.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.437	412	417	422	rBV	4236086	4630415	100.00%	23.163%
2	1.563	452	456	461	rBV	147291	80589	1.74%	0.403%
3	1.609	465	470	473	rBV	83310	47230	1.02%	0.236%
4	1.842	538	542	553	rBV	2388191	1681723	36.32%	8.413%
5	1.894	553	558	571	rVV	4025763	3049678	65.86%	15.256%
6	2.803	829	839	846	rBV	712204	738556	15.95%	3.695%
7	2.861	854	857	865	rVB	43377	46747	1.01%	0.234%
8	3.713	1116	1120	1134	rVB5	30476	49633	1.07%	0.248%
9	3.981	1189	1203	1217	rBV	874780	1350833	29.17%	6.757%
10	6.962	2112	2124	2141	rVB4	64305	129771	2.80%	0.649%
11	8.904	2709	2724	2734	rBV	1115640	1602124	34.60%	8.014%
12	8.959	2734	2741	2749	rVB4	34697	54772	1.18%	0.274%
13	9.173	2797	2807	2819	rBV3	258085	365761	7.90%	1.830%
14	9.237	2819	2827	2836	rVB3	62496	92926	2.01%	0.465%
15	9.377	2858	2870	2883	rBV	209408	290943	6.28%	1.455%
16	9.551	2912	2924	2943	rVB	690111	1199010	25.89%	5.998%
17	9.729	2973	2979	2998	rVB4	45798	81356	1.76%	0.407%
18	9.888	3015	3028	3036	rVB8	39809	62475	1.35%	0.313%
19	9.985	3045	3058	3073	rVB2	180812	271915	5.87%	1.360%
20	10.396	3166	3185	3194	rBV	1416105	1779084	38.42%	8.900%
21	10.875	3326	3333	3340	rVV4	60847	81020	1.75%	0.405%
22	10.921	3340	3347	3355	rVB8	33167	56874	1.23%	0.285%
23	11.111	3397	3406	3411	rBV3	44982	56216	1.21%	0.281%
24	11.218	3431	3439	3446	rVB6	39740	55937	1.21%	0.280%
25	11.552	3534	3542	3552	rVB4	88133	125469	2.71%	0.628%
26	11.769	3601	3609	3614	rBV3	109465	130420	2.82%	0.652%
27	12.060	3684	3699	3705	rBV	324407	344552	7.44%	1.724%
28	12.102	3705	3712	3719	rBV2	54836	59026	1.27%	0.295%
29	12.244	3748	3756	3760	rBV2	240585	282188	6.09%	1.412%
30	12.267	3760	3763	3778	rVB	196546	213297	4.61%	1.067%
31	12.458	3806	3822	3836	rBV2	217356	312572	6.75%	1.564%
32	12.523	3836	3842	3850	rBV4	86821	100675	2.17%	0.504%
33	12.662	3877	3885	3891	rBV2	130112	172131	3.72%	0.861%
34	12.840	3932	3940	3947	rBV3	60850	72537	1.57%	0.363%
35	12.892	3947	3956	3963	rVV2	109850	131067	2.83%	0.656%
36	12.943	3963	3972	3978	rVB4	46486	58290	1.26%	0.292%

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Instrument :
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ClientSampleId :
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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

37	13.008	3985	3992	4003	rBV5	43431	72665	1.57%	0.363%
38	13.400	4105	4113	4122	rVB2	52390	59964	1.30%	0.300%

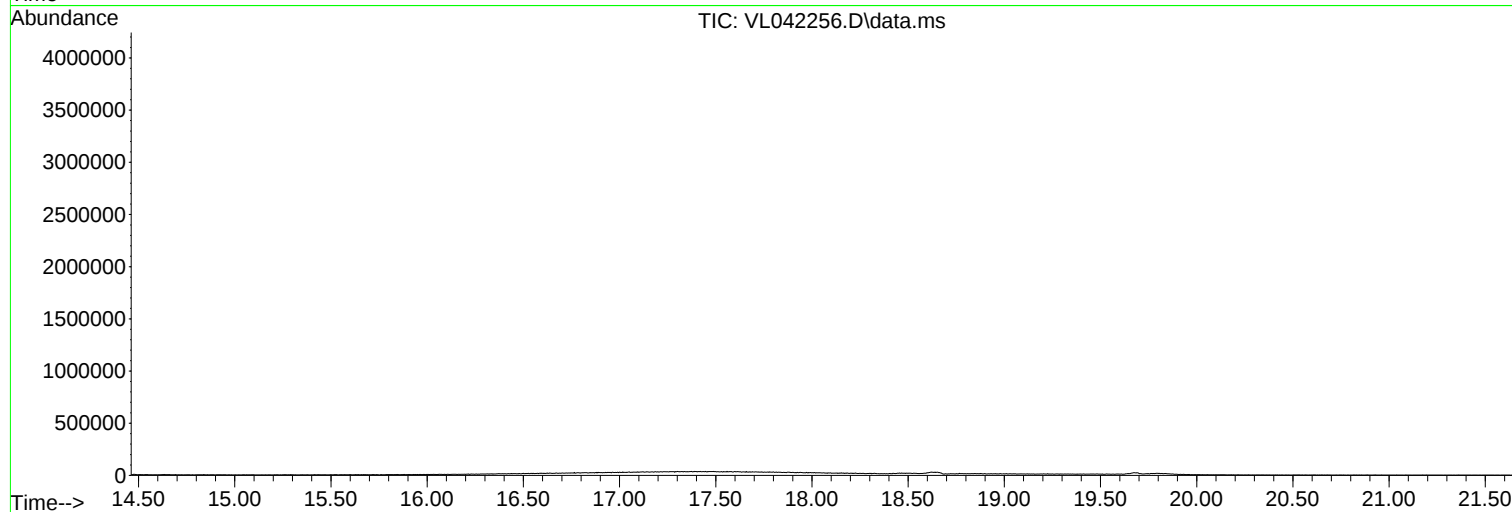
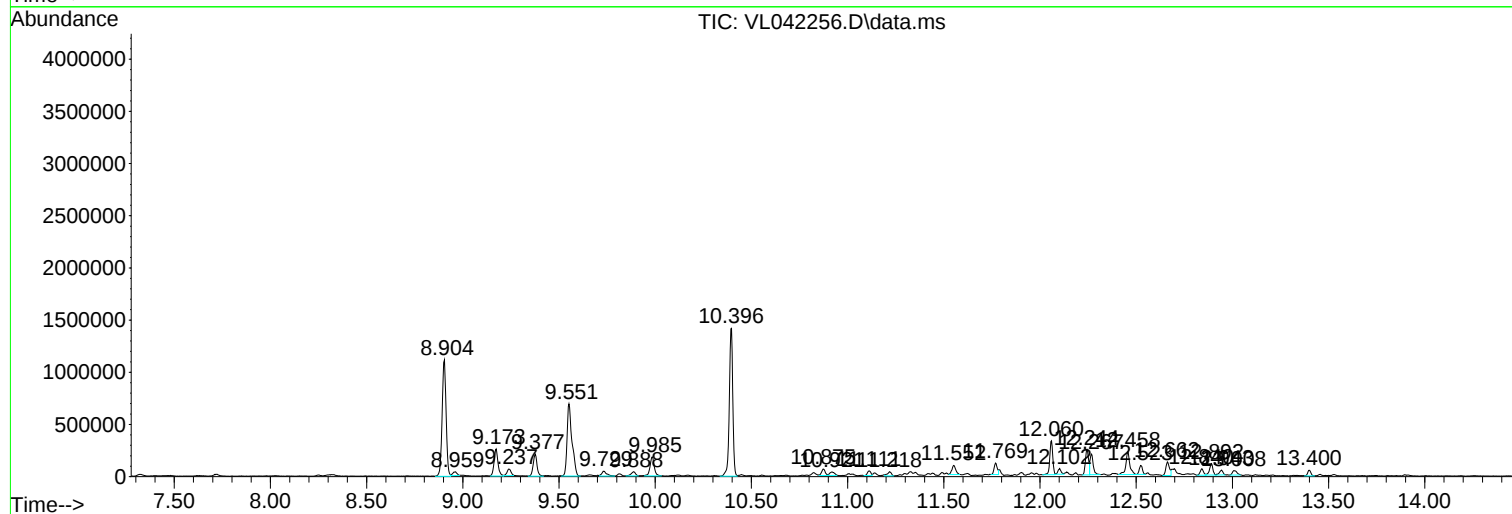
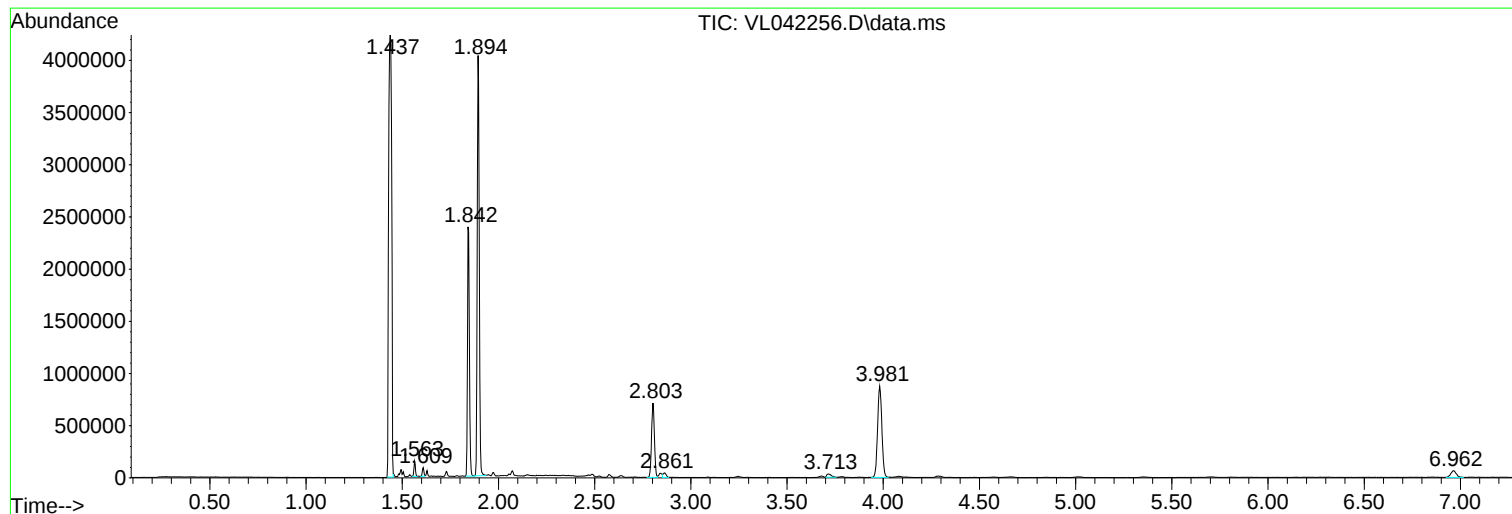
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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



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Instrument :
MSVOA_L
ClientSampleId :
SSSG-DUP-2-04012025

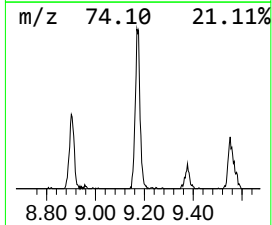
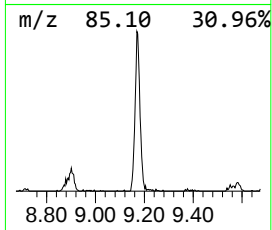
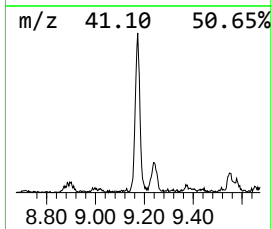
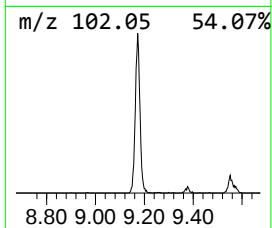
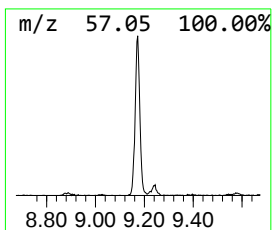
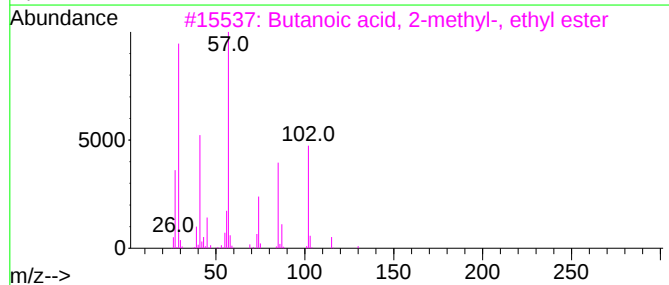
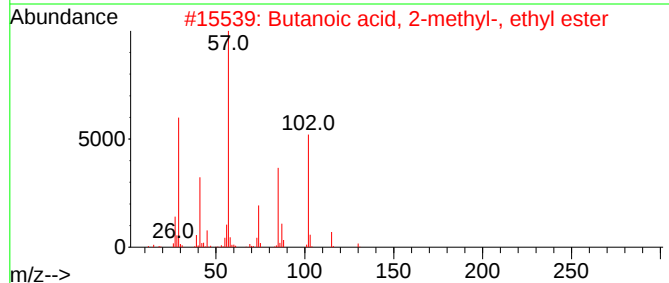
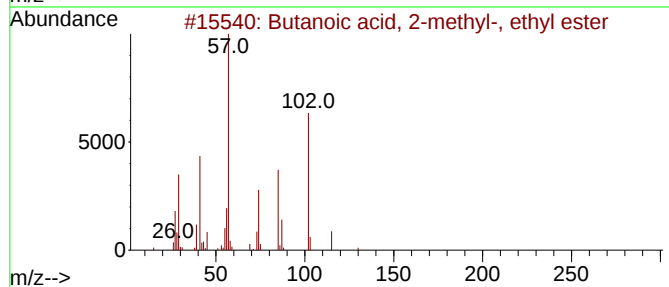
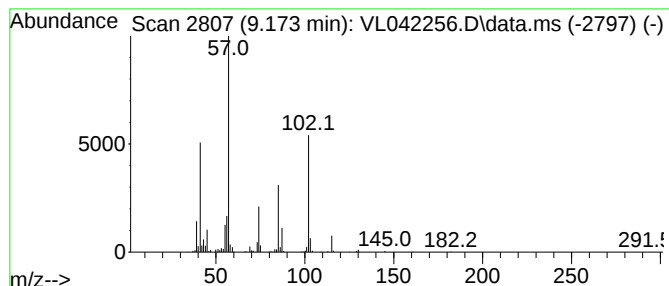
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 1 Butanoic acid, 2-methyl-, e... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.173	2.28 ppbv	365761	Chlorobenzene-d5	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	91
2			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	90
3			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	87
4			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	83
5			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	58



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

Instrument :
MSVOA_L
ClientSampleId :
SSSG-DUP-2-04012025

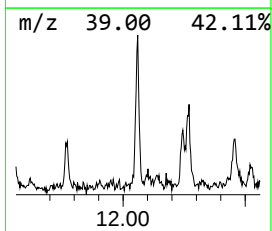
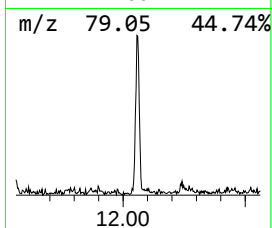
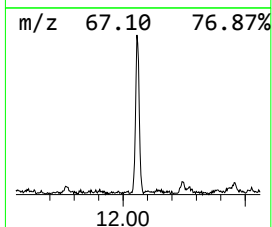
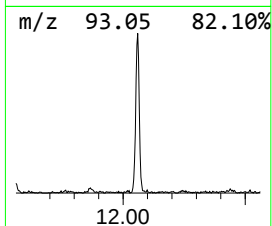
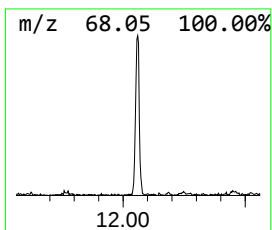
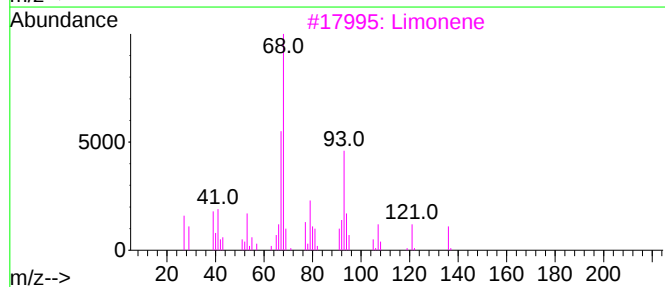
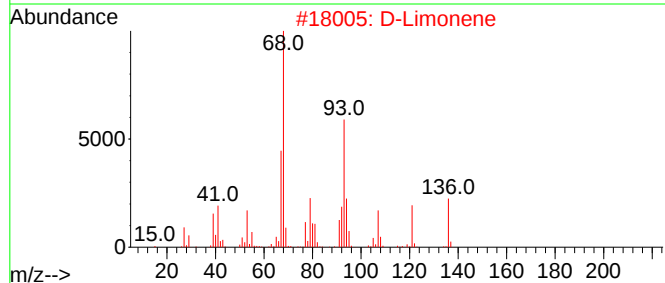
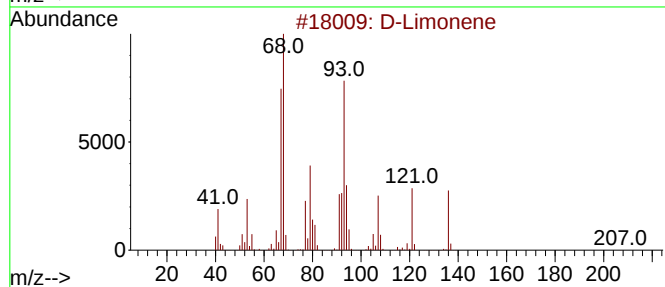
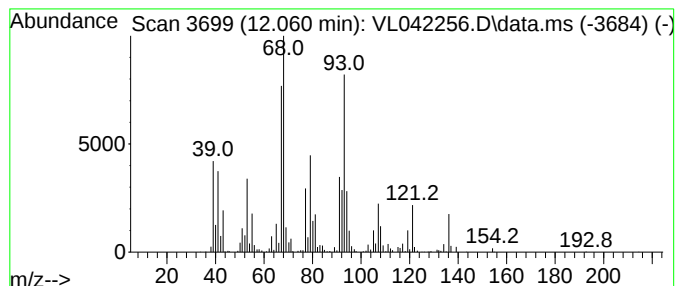
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 2 D-Limonene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	2.15 ppbv	344552	Chlorobenzene-d5	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Limonene			136	C10H16	005989-27-5	96
2	D-Limonene			136	C10H16	005989-27-5	94
3	Limonene			136	C10H16	000138-86-3	94
4	Limonene			136	C10H16	000138-86-3	94
5	D-Limonene			136	C10H16	005989-27-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_L\Data\VL040825\
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Sample : Q1725-03
Misc : 400mL/MSVOA_L
ALS Vial : 1 Sample Multiplier: 1

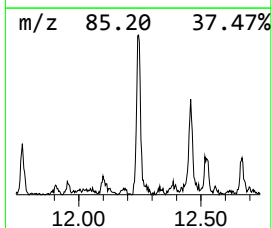
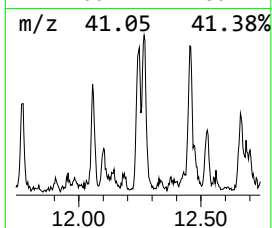
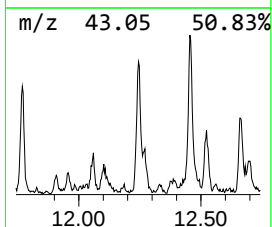
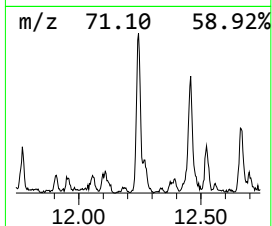
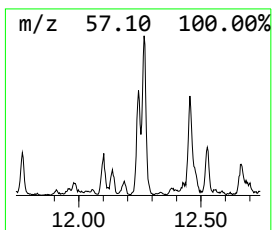
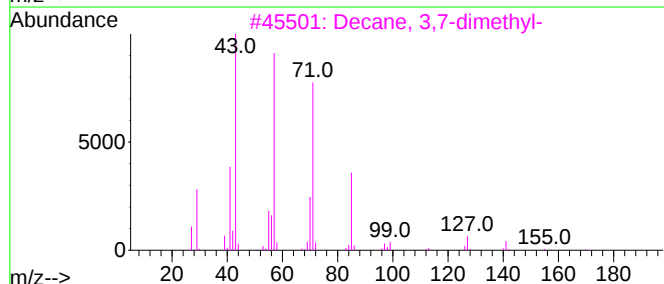
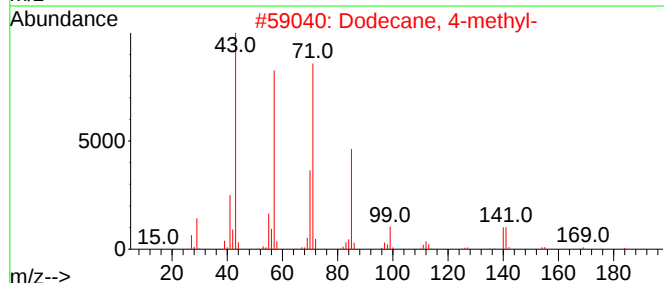
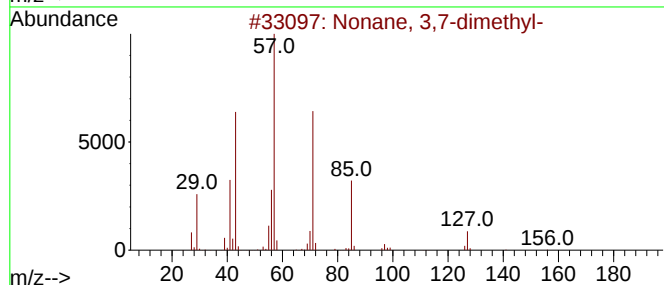
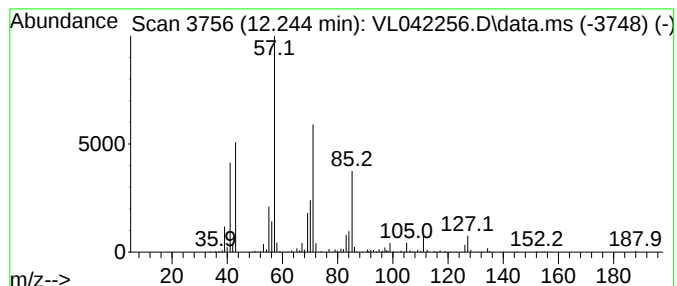
Instrument :
MSVOA_L
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 3 Nonane, 3,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.244	1.76 ppbv	282188	Chlorobenzene-d5	8.904	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	62
2	Dodecane, 4-methyl-	184	C13H28	006117-97-1	59
3	Decane, 3,7-dimethyl-	170	C12H26	017312-54-8	59
4	Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	53
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53



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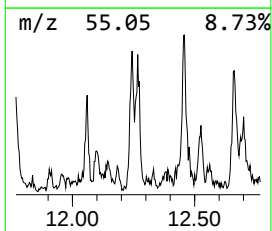
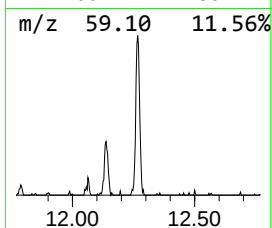
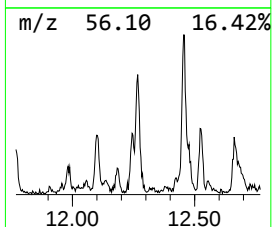
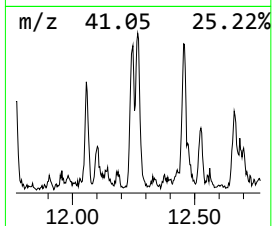
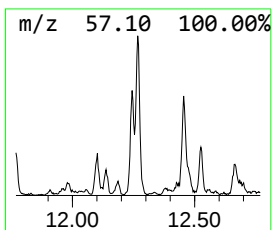
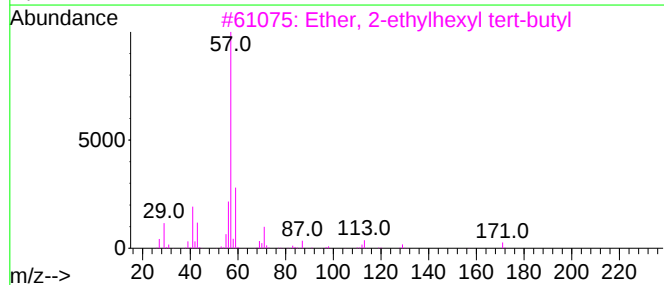
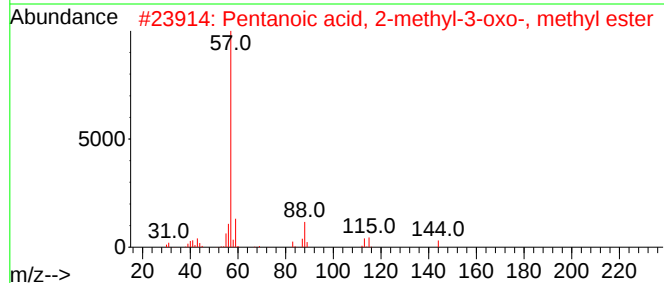
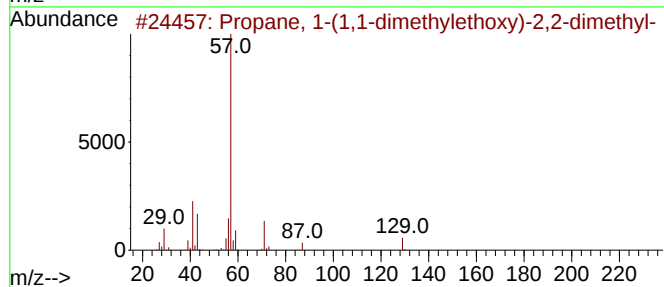
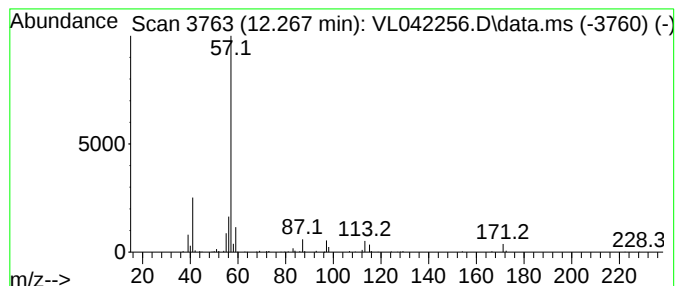
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.267 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.267	1.33 ppbv	213297	Chlorobenzene-d5	8.904	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-(1,1-dimethylethoxy)-...	144	C9H20O	032970-46-0	40
2	Pentanoic acid, 2-methyl-3-oxo-,...	144	C7H12O3	017422-12-7	40
3	Ether, 2-ethylhexyl tert-butyl	186	C12H26O	083704-03-4	33
4	Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	12
5	Oxalic acid, isobutyl heptyl ester	244	C13H24O4	1000309-37-2	12



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MSVOA_L
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SSSG-DUP-2-04012025

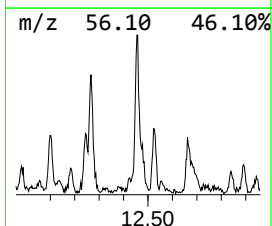
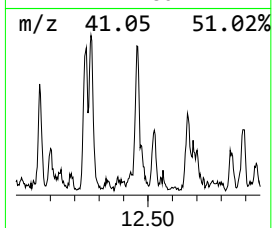
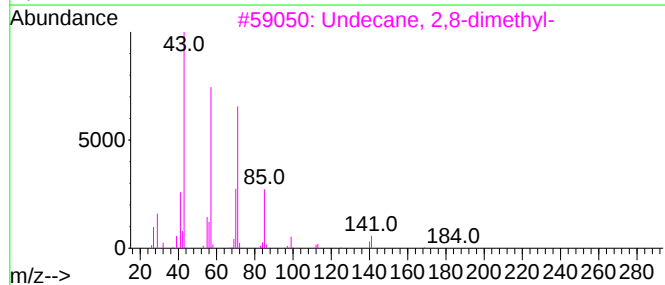
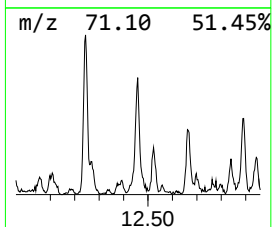
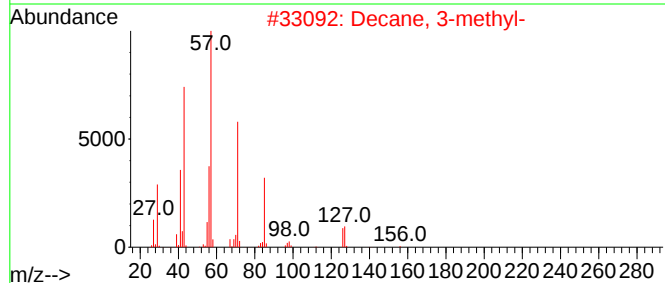
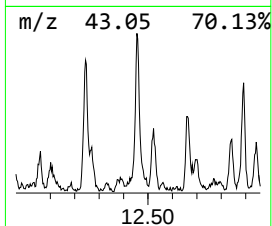
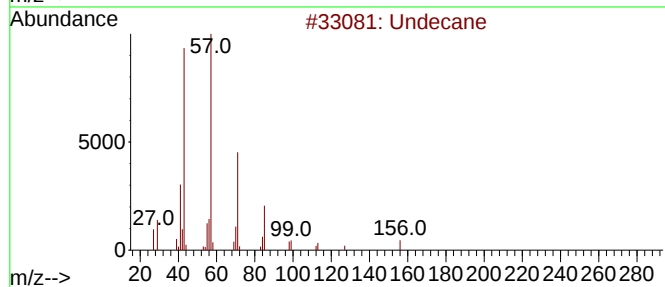
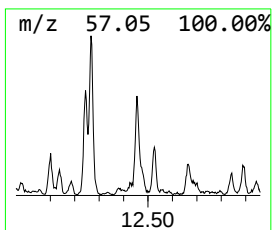
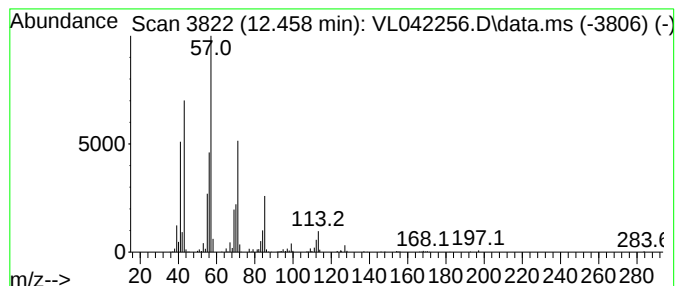
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 5 Undecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.458	1.95 ppbv	312572	Chlorobenzene-d5	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	53
2	Decane, 3-methyl-			156	C11H24	013151-34-3	47
3	Undecane, 2,8-dimethyl-			184	C13H28	017301-25-6	47
4	Nonane, 3-methyl-			142	C10H22	005911-04-6	47
5	Oxalic acid, butyl 2-ethylhexyl ...			258	C14H26O4	1000309-38-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_L\Data\VL040825\
Data File : VL042256.D
Acq On : 08 Apr 2025 10:55
Operator : SY/MD
Sample : Q1725-03
Misc : 400mL/MSVOA_L
ALS Vial : 1 Sample Multiplier: 1

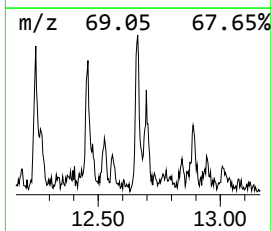
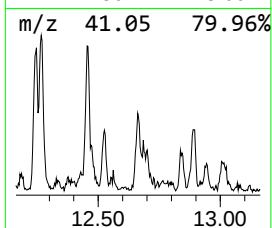
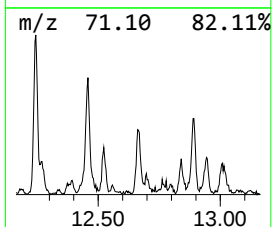
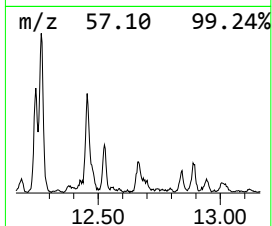
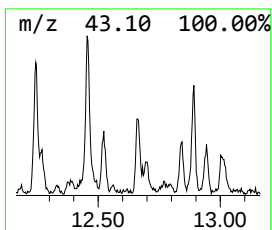
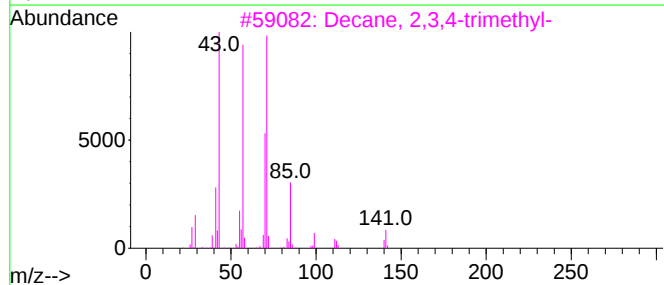
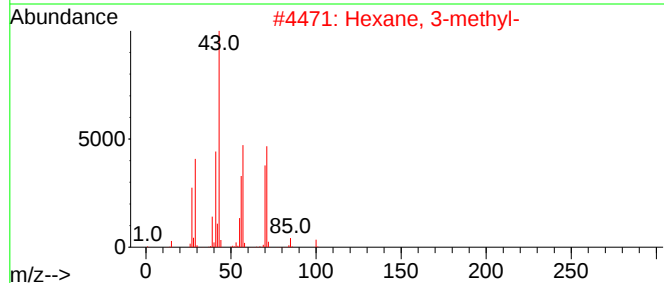
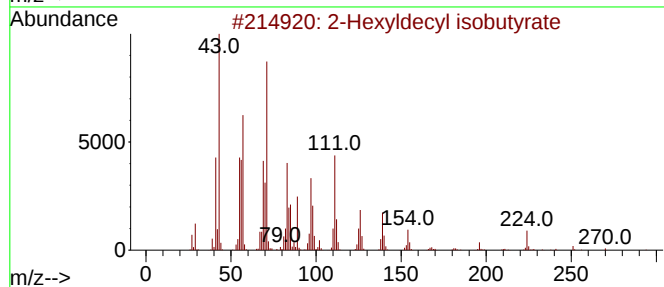
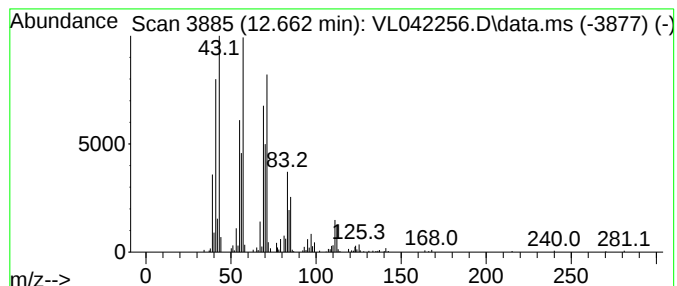
Instrument :
MSVOA_L
ClientSampleId :
SSSG-DUP-2-04012025

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 2-Hexyldecyl isobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.662	1.07 ppbv	172131	Chlorobenzene-d5		8.904	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Hexyldecyl isobutyrate		312	C20H40O2	1000368-55-3	64
2	Hexane, 3-methyl-		100	C7H16	000589-34-4	50
3	Decane, 2,3,4-trimethyl-		184	C13H28	062238-15-7	47
4	Butane, 2,2-dimethyl-		86	C6H14	000075-83-2	43
5	Heptane, 3-ethyl-5-methyl-		142	C10H22	052896-90-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_L\Data\VL040825\
Data File : VL042256.D
Acq On : 08 Apr 2025 10:55
Operator : SY/MD
Sample : Q1725-03
Misc : 400mL/MSVOA_L
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_L
ClientSampleId :
SSSG-DUP-2-04012025

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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanoic acid, ...	9.173	2.3	ppbv	365761	3	8.904	1602120	10.0
D-Limonene	12.060	2.1	ppbv	344552	3	8.904	1602120	10.0
Nonane, 3,7-dim...	12.244	1.8	ppbv	282188	3	8.904	1602120	10.0
unknown12.267	12.267	1.3	ppbv	213297	3	8.904	1602120	10.0
Undecane	12.458	2.0	ppbv	312572	3	8.904	1602120	10.0
2-Hexyldecyl is...	12.662	1.1	ppbv	172131	3	8.904	1602120	10.0