

Data Path : Z:\voasrv\HPCHEM1\MSVOA_L\Data\VL040825\
 Data File : VL042277.D
 Acq On : 08 Apr 2025 23:44
 Operator : SY/MD
 Sample : Q1728-01 2X
 Misc : 400mL/MSVOA_L
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_L
 ClientSampleId :
 SSSG-B14-2-04012025

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: VL042277.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	411	416	421	rBV	4092978	4481916	100.00%	32.385%
2	1.560	451	455	459	rBV2	118010	66513	1.48%	0.481%
3	1.839	536	541	552	rBV	1450572	944257	21.07%	6.823%
4	1.890	552	557	570	rVB	2472701	1774519	39.59%	12.822%
5	2.065	607	611	620	rVB	118214	91072	2.03%	0.658%
6	2.793	828	836	843	rBV	575759	606914	13.54%	4.385%
7	2.835	843	849	863	rVB4	64885	90726	2.02%	0.656%
8	3.968	1185	1199	1213	rBV	720897	1107989	24.72%	8.006%
9	6.949	2107	2120	2130	rBV3	46750	96976	2.16%	0.701%
10	8.891	2705	2720	2730	rBV	902653	1301589	29.04%	9.405%
11	8.949	2730	2738	2747	rVB3	54898	88346	1.97%	0.638%
12	9.160	2792	2803	2814	rBV3	102374	157447	3.51%	1.138%
13	9.228	2814	2824	2835	rVB3	55477	82802	1.85%	0.598%
14	9.364	2855	2866	2880	rBV	57645	88218	1.97%	0.637%
15	9.538	2911	2920	2938	rVB2	157178	300800	6.71%	2.173%
16	9.720	2967	2976	2987	rBV3	30796	48514	1.08%	0.351%
17	9.969	3045	3053	3071	rVB2	51128	87681	1.96%	0.634%
18	10.383	3162	3181	3191	rBV	1155547	1401209	31.26%	10.125%
19	10.866	3322	3330	3337	rBV4	35615	44898	1.00%	0.324%
20	11.545	3530	3540	3550	rVB4	29244	49092	1.10%	0.355%
21	11.781	3597	3613	3621	rVB4	100572	169382	3.78%	1.224%
22	12.047	3689	3695	3702	rVB4	51594	56839	1.27%	0.411%
23	12.235	3744	3753	3757	rBV	151512	177857	3.97%	1.285%
24	12.257	3757	3760	3771	rVB	144128	158930	3.55%	1.148%
25	12.448	3811	3819	3833	rVB3	102641	146682	3.27%	1.060%
26	12.516	3833	3840	3847	rBV3	44357	53177	1.19%	0.384%
27	12.655	3874	3883	3887	rBV5	54487	69309	1.55%	0.501%
28	12.833	3929	3938	3945	rBV3	36996	46037	1.03%	0.333%
29	12.882	3945	3953	3960	rVB2	41278	49904	1.11%	0.361%

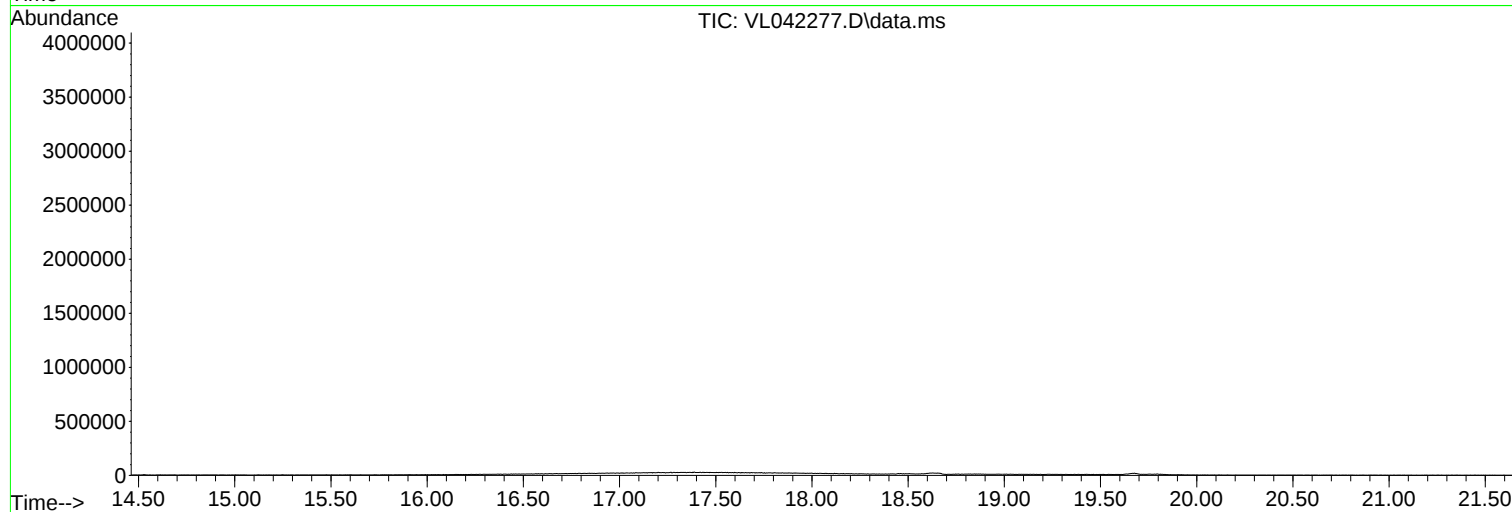
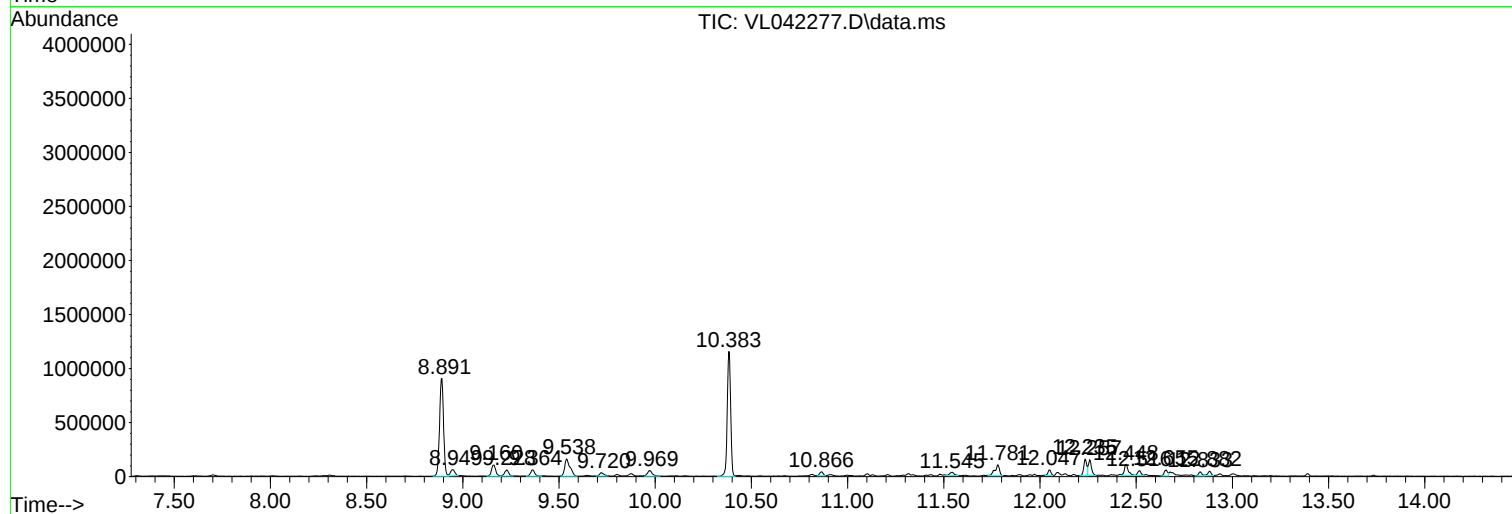
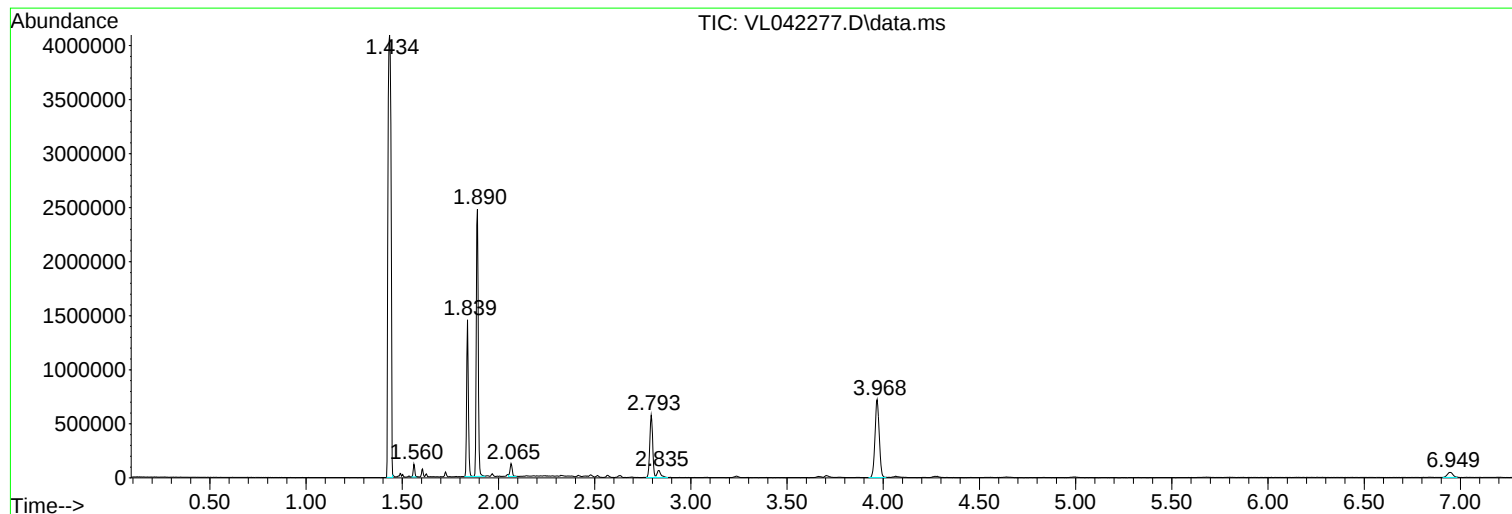
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Instrument :
MSVOA_L
ClientSampleId :
SSSG-B14-2-04012025

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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SSSG-B14-2-04012025

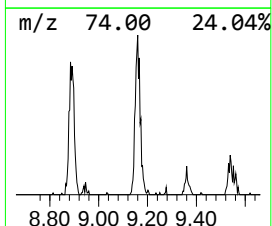
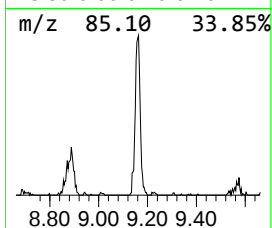
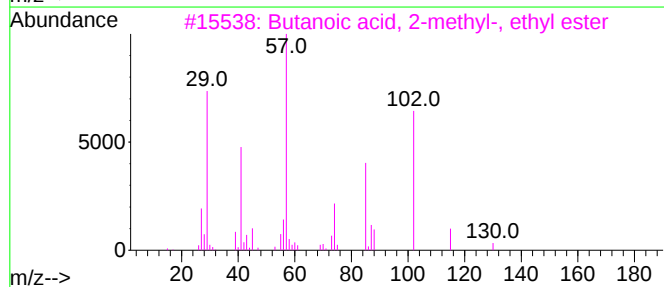
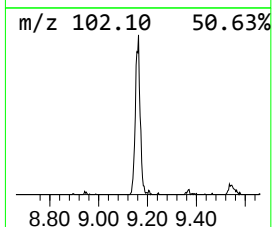
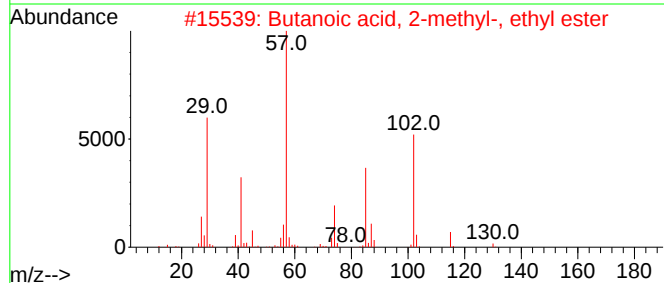
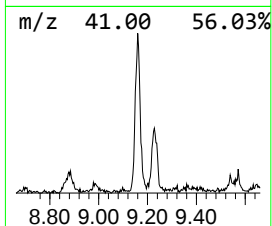
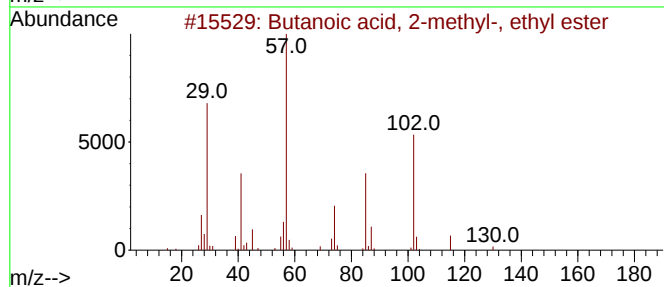
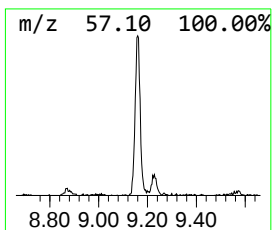
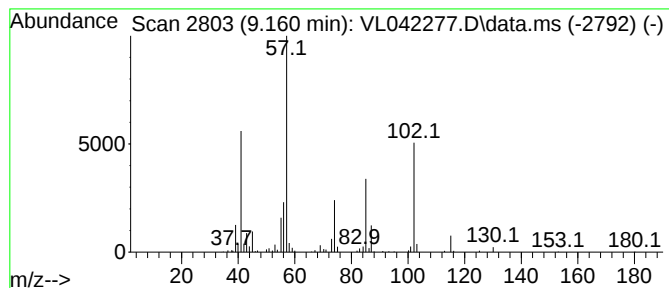
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 1 Butanoic acid, 2-methyl-, e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.160	1.21 ppbv	157447	Chlorobenzene-d5	8.891

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	90
2			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	74
3			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	58
4			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	53
5			Butanoic acid, 2-methyl-, ethyl ...	130	C7H14O2	007452-79-1	50



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

Instrument :
MSVOA_L
ClientSampleId :
SSSG-B14-2-04012025

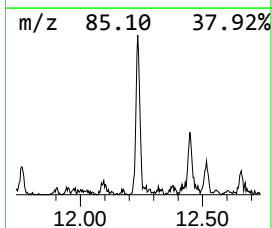
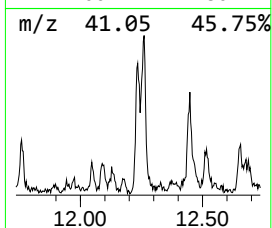
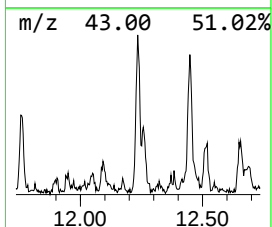
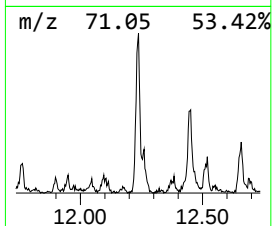
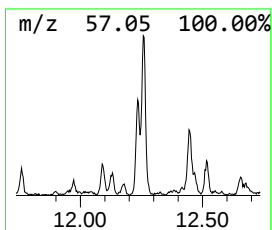
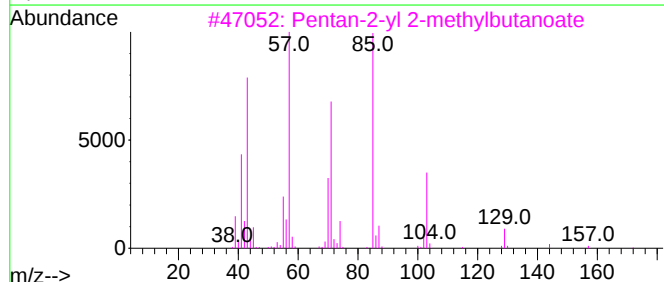
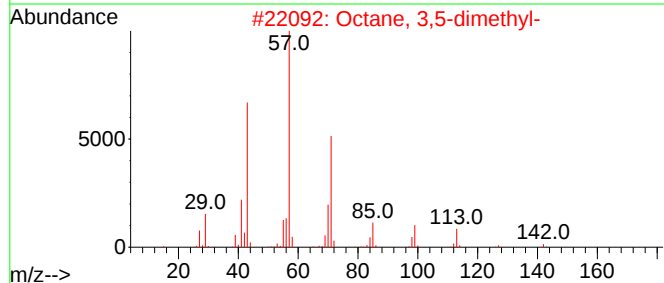
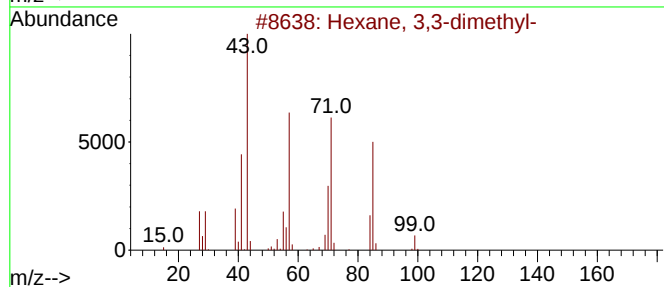
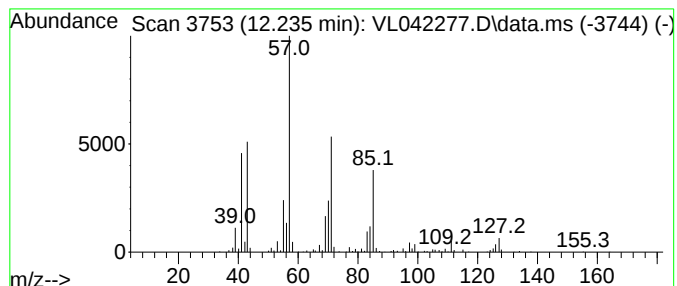
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

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

Peak Number 3 Hexane, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.235	1.37 ppbv	177857	Chlorobenzene-d5	8.891

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
2			Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	53
3			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	53
4			Dodecane, 4-methyl-	184	C13H28	006117-97-1	53
5			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	50



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SSSG-B14-2-04012025

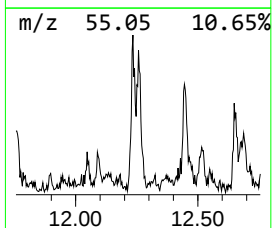
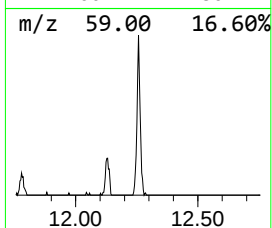
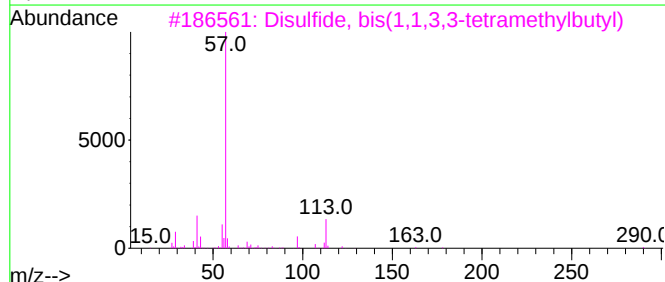
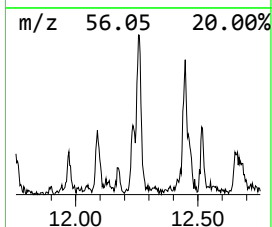
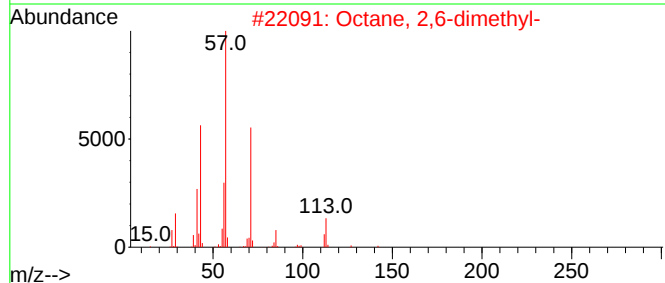
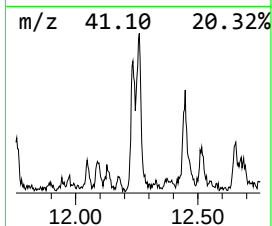
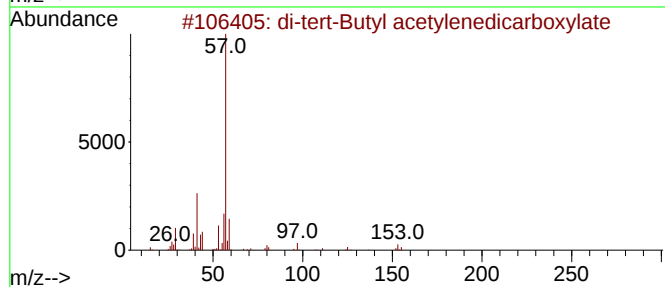
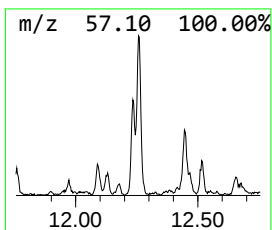
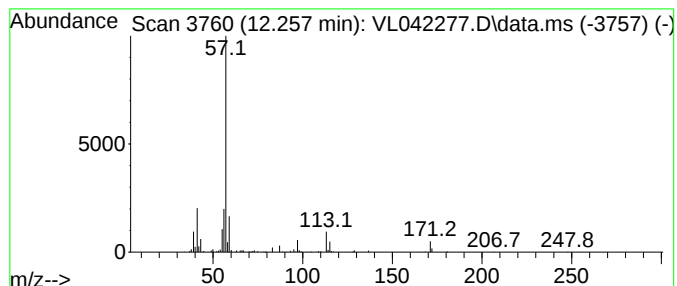
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL032725AIR.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.257 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.257	1.22 ppbv	158930	Chlorobenzene-d5	8.891

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			di-tert-Butyl acetylenedicarboxy...	226	C12H18O4	066086-33-7	40
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	32
3			Disulfide, bis(1,1,3,3-tetrameth...	290	C16H34S2	029956-99-8	32
4			sec-Butyl isobutyl carbonate	174	C9H18O3	1000372-77-3	28
5			Glycerol, 2-tert-butyl ether	148	C7H16O3	1000381-76-3	28



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ALS Vial : 1 Sample Multiplier: 1

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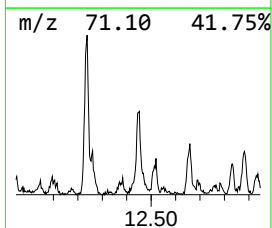
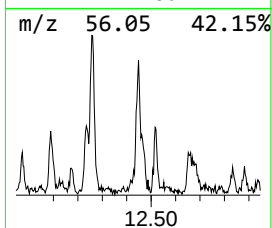
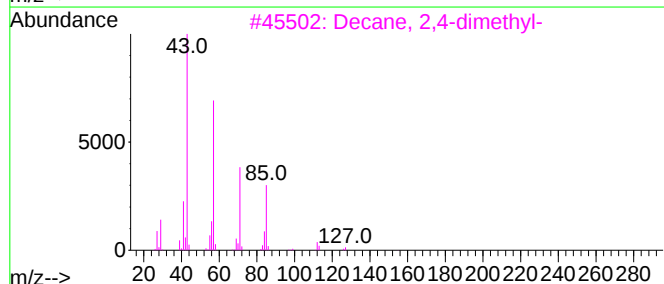
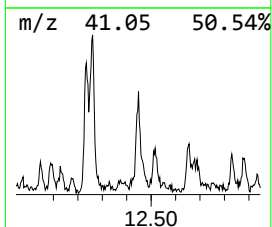
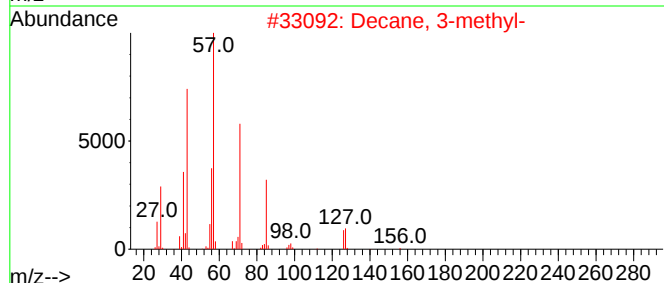
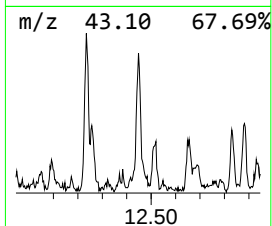
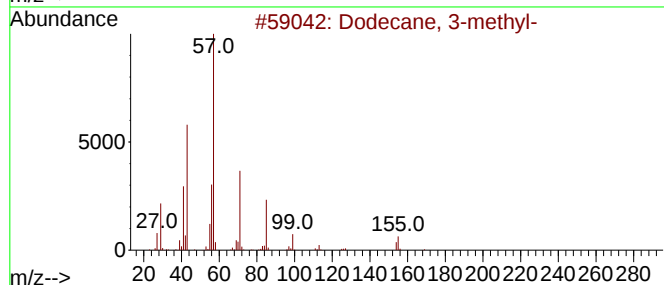
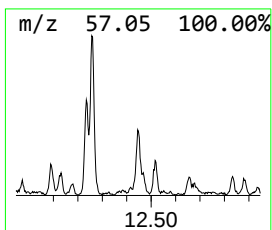
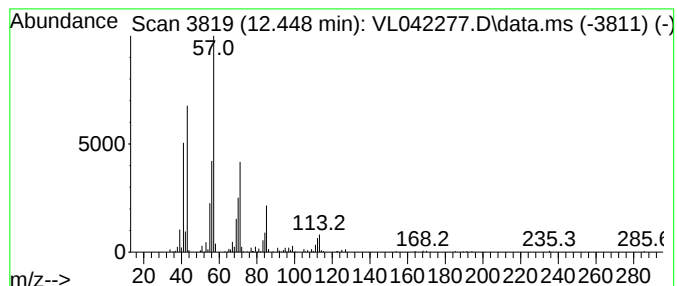
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dodecane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.448	1.13 ppbv	146682	Chlorobenzene-d5	8.891

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 3-methyl-	184	C13H28	017312-57-1	59
2			Decane, 3-methyl-	156	C11H24	013151-34-3	50
3			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	50
4			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	50
5			Decane, 3,6-dimethyl-	170	C12H26	017312-53-7	49



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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, ...	9.160	1.2	ppbv	157447	3	8.891	1301590	10.0
Hexane, 3,3-dim...	12.235	1.4	ppbv	177857	3	8.891	1301590	10.0
unknown12.257	12.257	1.2	ppbv	158930	3	8.891	1301590	10.0
Dodecane, 3-met...	12.448	1.1	ppbv	146682	3	8.891	1301590	10.0