

Data Path : Z:\voasrv\HPCHEM1\MSVOA_L\Data\VL102522\
 Data File : VL039792.D
 Acq On : 25 Oct 2022 17:53
 Operator : SY/AP
 Sample : N5227-12
 Misc : 400mL/MSVOA_L
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_L
 ClientSampleId :
 L

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\VL102422AIR.M

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

Signal : TIC: VL039792.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.661	11	18	25	rVB2	4955717	5372288	58.53%	9.182%
2	2.690	25	27	39	rVB4	1111337	1473389	16.05%	2.518%
3	2.732	39	40	50	rVB4	414018	382384	4.17%	0.654%
4	2.822	50	68	83	rBV4	1565313	3691441	40.22%	6.309%
5	2.893	87	90	99	rVB2	212665	226521	2.47%	0.387%
6	2.957	103	110	116	rVB3	180522	206297	2.25%	0.353%
7	2.999	116	123	129	rBV2	126903	175494	1.91%	0.300%
8	3.034	129	134	144	rVB	245642	338128	3.68%	0.578%
9	3.089	144	151	159	rBV3	155987	217726	2.37%	0.372%
10	3.205	182	187	196	rBV5	74774	97020	1.06%	0.166%
11	3.279	196	210	218	rVB5	122841	268158	2.92%	0.458%
12	3.350	224	232	242	rVB2	183204	262255	2.86%	0.448%
13	3.488	268	275	281	rBV	413705	636283	6.93%	1.087%
14	3.510	281	282	297	rVB3	303389	313875	3.42%	0.536%
15	3.751	350	357	366	rBV2	217611	320688	3.49%	0.548%
16	3.838	376	384	393	rVB4	88168	144479	1.57%	0.247%
17	3.951	407	419	453	rBV	5238347	9178787	100.00%	15.687%
18	4.160	472	484	499	rBV10	109728	246714	2.69%	0.422%
19	4.674	635	644	656	rVB6	75472	145259	1.58%	0.248%
20	4.922	710	721	732	rBV7	52897	95281	1.04%	0.163%
21	5.224	793	815	849	rBV3	3188844	8766160	95.50%	14.982%
22	6.661	1248	1262	1282	rBV	2898181	5773592	62.90%	9.868%
23	6.729	1282	1283	1299	rVB5	80346	109885	1.20%	0.188%
24	8.253	1744	1757	1768	rBV9	59437	128806	1.40%	0.220%
25	9.230	2058	2061	2073	rVB3	74267	96526	1.05%	0.165%
26	10.150	2332	2347	2367	rBV5	192378	438688	4.78%	0.750%
27	11.063	2617	2631	2643	rBV5	281812	598024	6.52%	1.022%
28	11.468	2739	2757	2783	rBV	2903578	6871658	74.86%	11.744%
29	13.777	3455	3475	3508	rBV2	2750187	7141917	77.81%	12.206%
30	15.249	3916	3933	3953	rBV2	279952	732976	7.99%	1.253%
31	15.452	3978	3996	4009	rBV10	238899	727690	7.93%	1.244%
32	15.536	4009	4022	4041	rVB5	587625	1528216	16.65%	2.612%
33	16.365	4267	4280	4281	rBV10	84799	94317	1.03%	0.161%
34	16.378	4281	4284	4300	rVB4	106345	179932	1.96%	0.308%
35	16.481	4304	4316	4326	rBV4	40327	92768	1.01%	0.159%
36	17.185	4516	4535	4556	rBV4	229102	770609	8.40%	1.317%

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Instrument :
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ClientSampleId :
L

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\VL102422AIR.M
Title : AIR ANALYSIS BY METHOD TO-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

37	17.291	4556	4568	4582	rVB4	42066	108780	1.19%	0.186%
38	17.500	4616	4633	4634	rBV5	111031	166379	1.81%	0.284%
39	20.796	5639	5658	5660	rBV2	133556	231344	2.52%	0.395%
40	20.805	5660	5661	5677	rVB	120843	160292	1.75%	0.274%

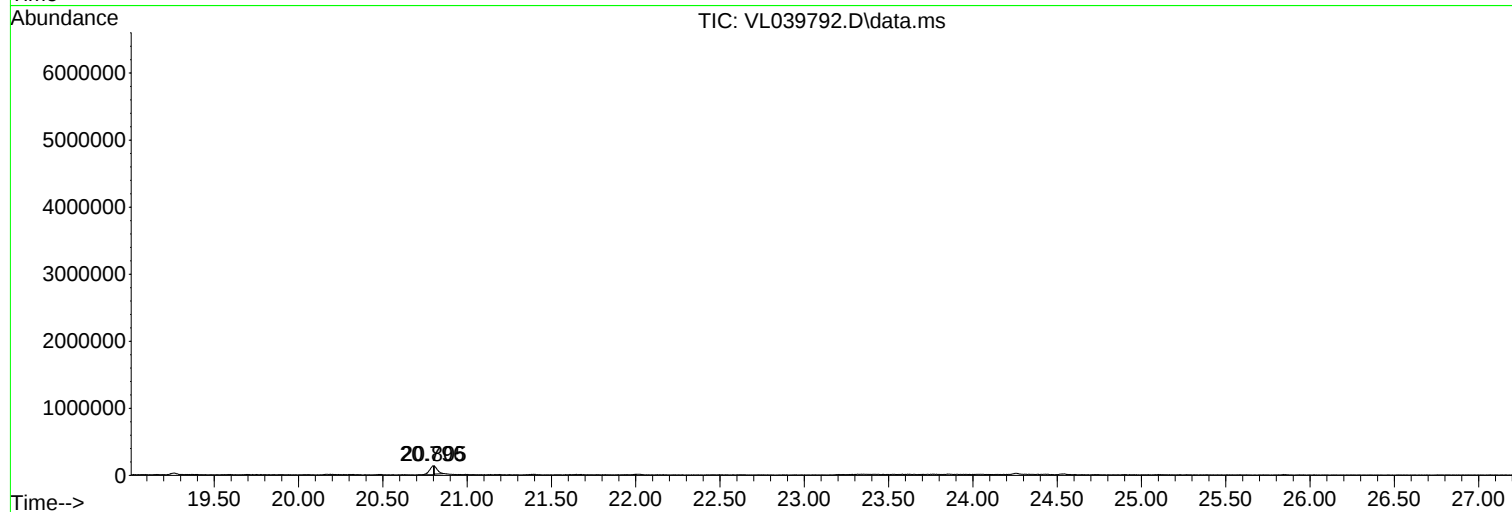
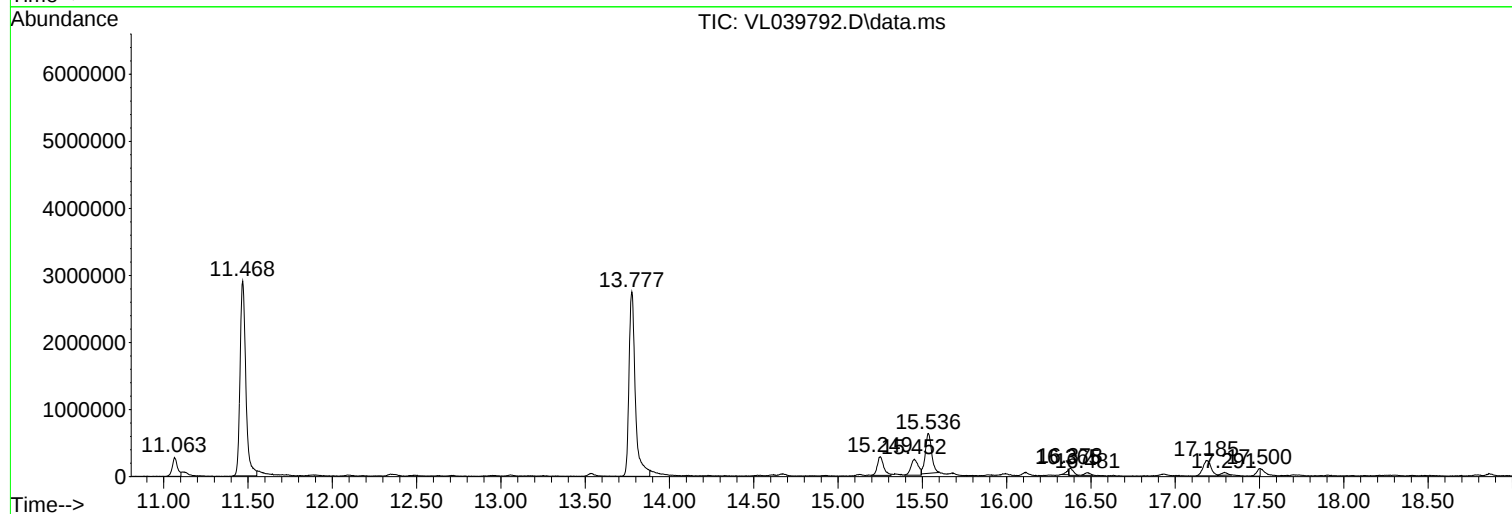
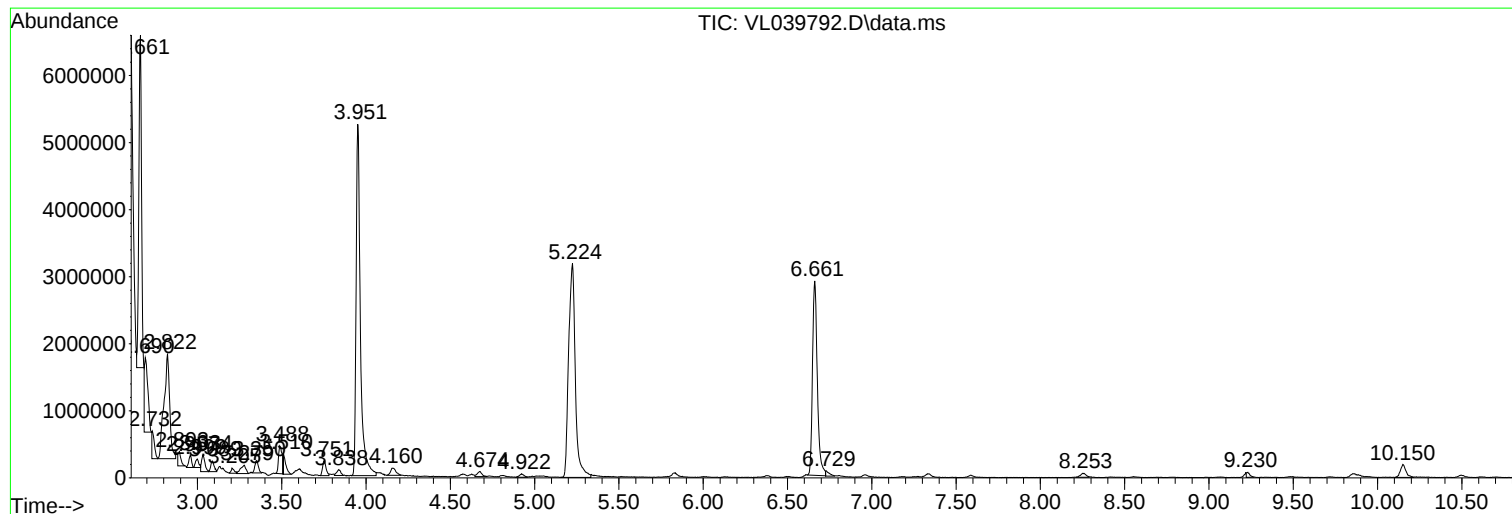
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL102422AIR.M
Quant Title : AIR ANALYSIS BY METHOD TO-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_L
ClientSampleId :
L

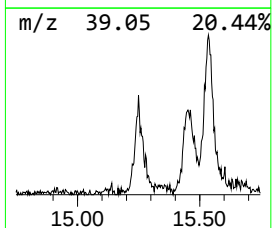
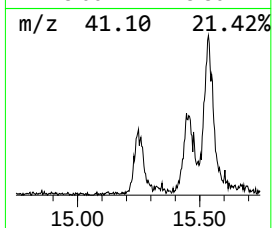
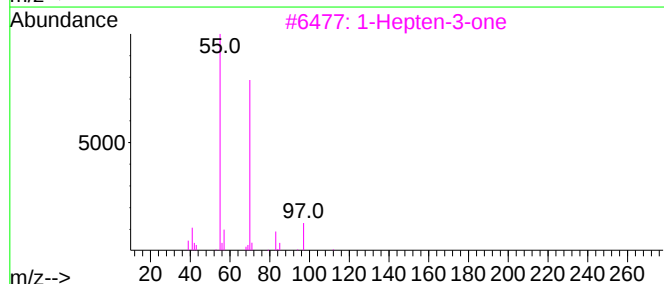
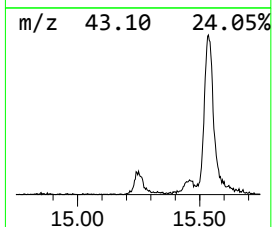
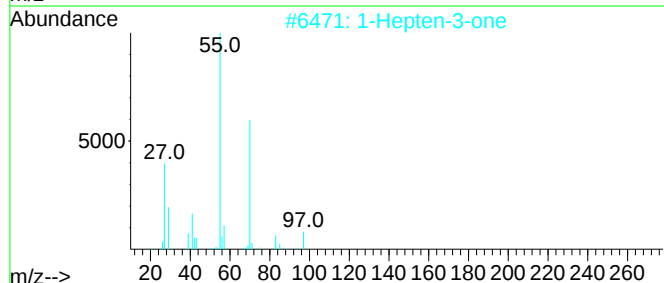
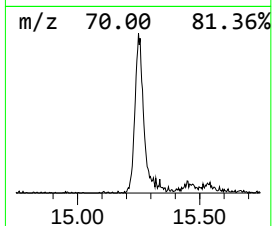
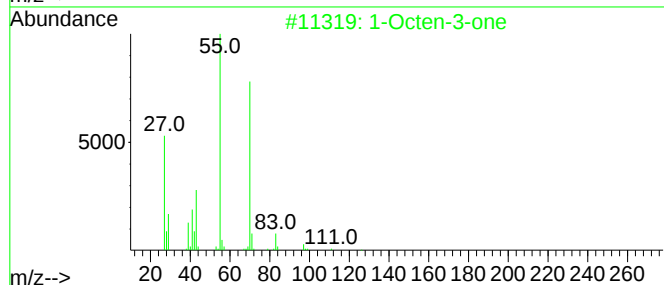
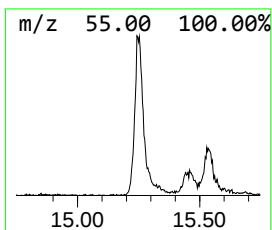
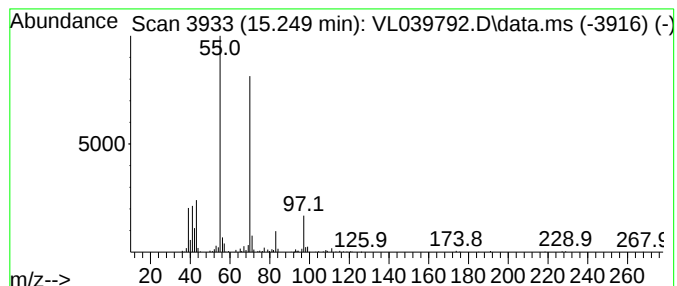
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL102422AIR.M
Quant Title : AIR ANALYSIS BY METHOD T0-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Octen-3-one Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.249	1.07 ppbv	732976	Chlorobenzene-d5	11.468

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Octen-3-one	126	C8H14O	004312-99-6	72
2		1-Hepten-3-one	112	C7H12O	002918-13-0	72
3		1-Hepten-3-one	112	C7H12O	002918-13-0	64
4		1-Butanol, 3-methyl-, formate	116	C6H12O2	000110-45-2	59
5		1,2-Cyclopentanedione, 3,3,5,5-t...	154	C9H14O2	020633-06-1	53



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Sample : N5227-12
Misc : 400mL/MSVOA_L
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_L
ClientSampleId :
L

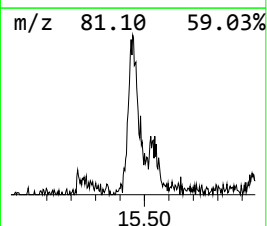
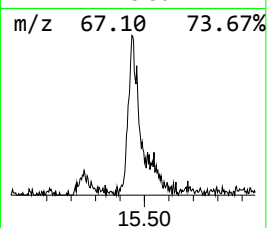
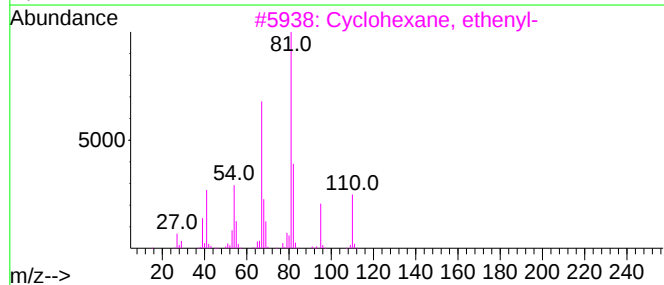
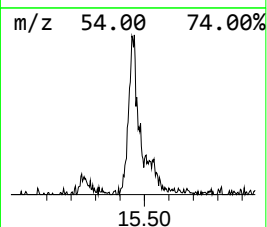
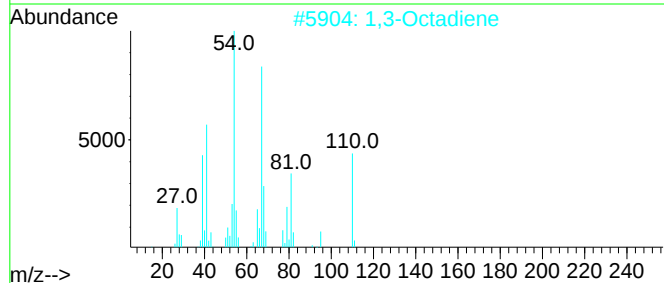
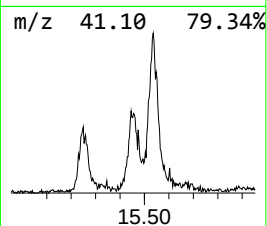
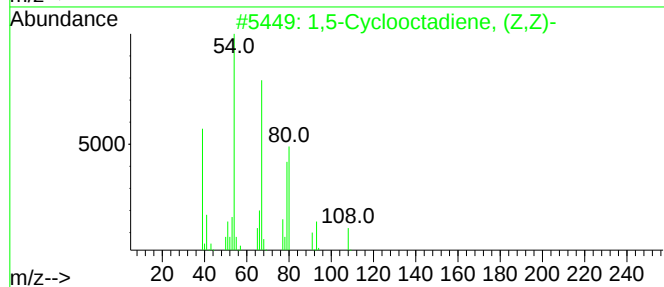
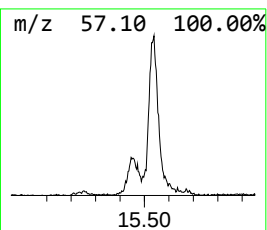
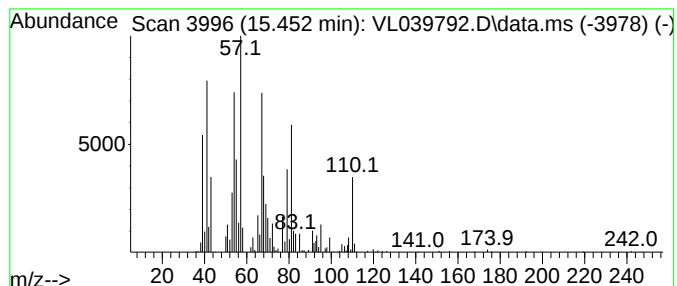
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL102422AIR.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,5-Cyclooctadiene, (Z,Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.452	1.06 ppbv	727690	Chlorobenzene-d5	11.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Cyclooctadiene, (Z,Z)-	108	C8H12	001552-12-1	90
2			1,3-Octadiene	110	C8H14	001002-33-1	87
3			Cyclohexane, ethenyl-	110	C8H14	000695-12-5	83
4			Cyclooctene	110	C8H14	000931-88-4	83
5			Cyclooctene	110	C8H14	000931-88-4	81



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

Instrument :
MSVOA_L
ClientSampleId :
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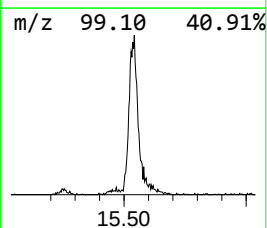
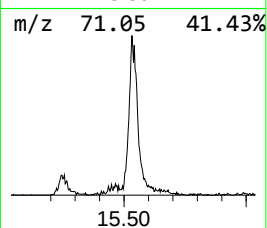
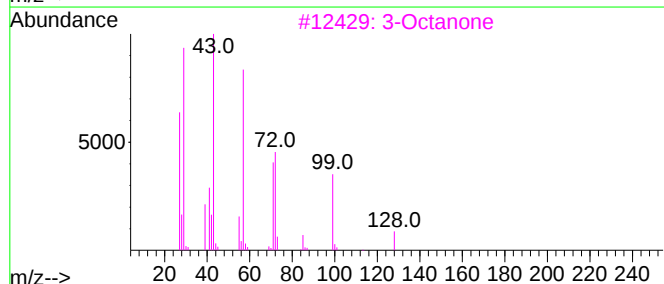
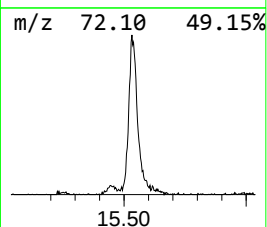
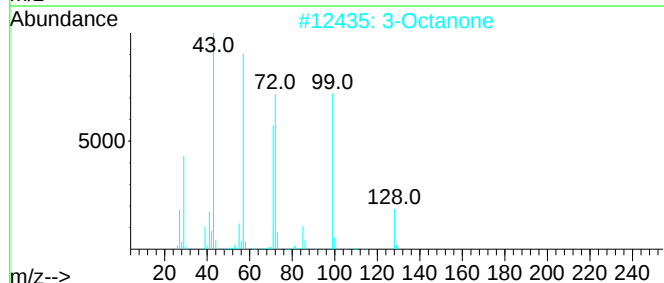
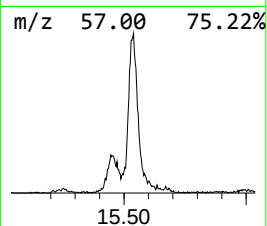
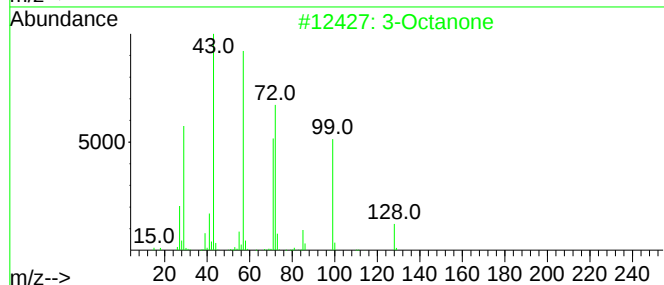
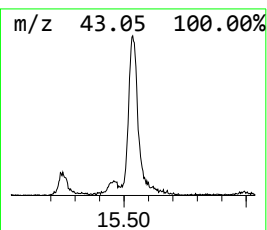
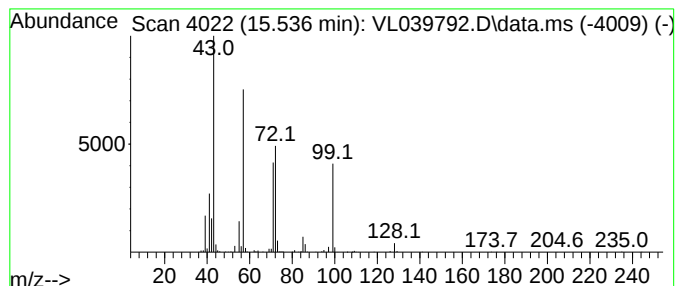
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_L\methods\VL102422AIR.M
Quant Title : AIR ANALYSIS BY METHOD TO-15 Instrument: MSVOA_L Fri Aug 26 06:05:16 2022

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.536	2.22 ppbv	1528220	Chlorobenzene-d5	11.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanone	128	C8H16O	000106-68-3	78
2			3-Octanone	128	C8H16O	000106-68-3	76
3			3-Octanone	128	C8H16O	000106-68-3	74
4			4-Oxononanal	156	C9H16O2	1000314-10-4	56
5			3-Octanone	128	C8H16O	000106-68-3	50



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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_L
ClientSampleId :
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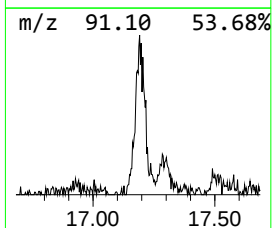
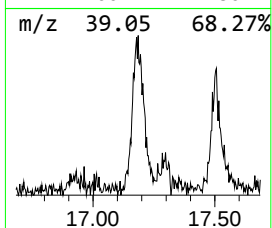
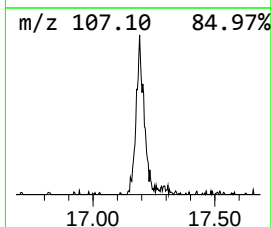
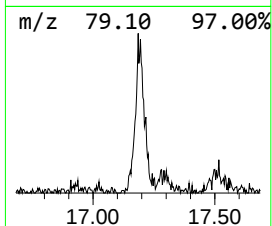
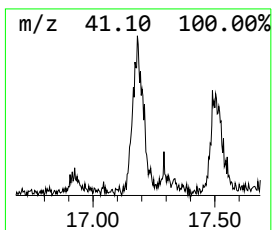
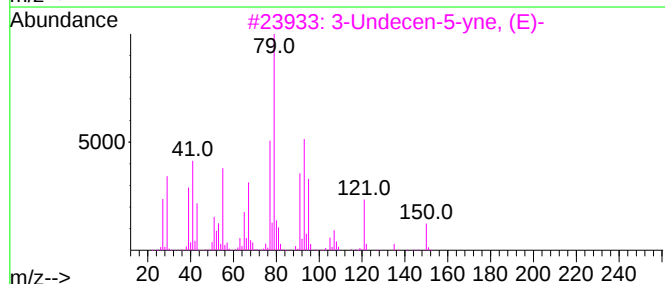
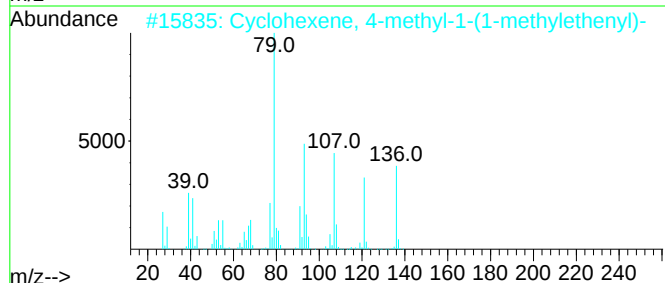
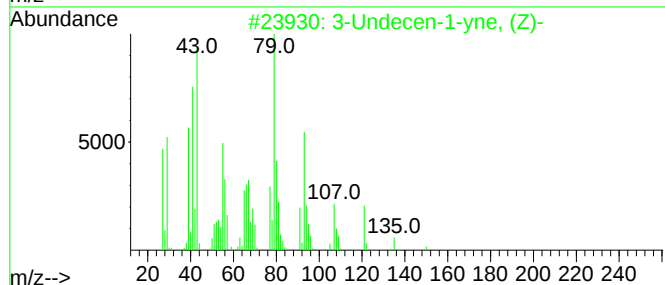
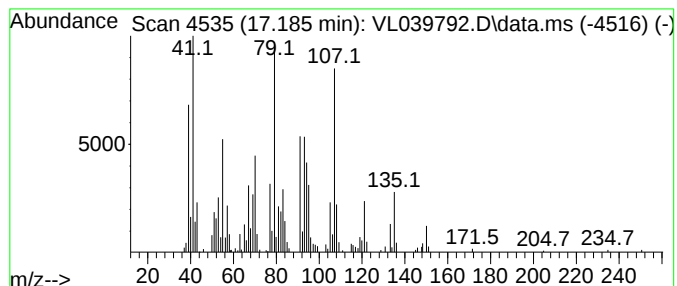
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown17.185 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.185	1.12 ppbv	770609	Chlorobenzene-d5	11.468

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3	Undecen-1-yne, (Z)-	150	C11H18	074744-32-4	49	
2	Cyclohexene, 4-methyl-1-(1-methy...	136	C10H16	000586-67-4	43		
3	3-Undecen-5-yne, (E)-	150	C11H18	074744-29-9	38		
4	Cyclopropane, (1-methyl-1,2-prop...	94	C7H10	051549-86-1	38		
5	Tricyclo[4.1.0.0(2,7)]heptane	94	C7H10	000287-13-8	38		



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Octen-3-one	15.249	1.1	ppbv	732976	3	11.468	6871660	10.0
1,5-Cyclooctadi...	15.452	1.1	ppbv	727690	3	11.468	6871660	10.0
3-Octanone	15.536	2.2	ppbv	1528220	3	11.468	6871660	10.0
unknown17.185	17.185	1.1	ppbv	770609	3	11.468	6871660	10.0