

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100220\
 Data File : VX018757.D
 Acq On : 02 Oct 2020 19:05
 Operator : JC/SP
 Sample : L4239-04
 Misc : 25.0mL/MSVOA X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BG3N3

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_X\METHOD\SOMXTR100220WMA.M
 Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.154	326	339	358	rBV	6074324	14121179	2.17%	0.673%
2	3.501	386	396	412	rVB	5036286	11550756	1.77%	0.550%
3	4.385	519	541	556	rBV	15092302	46359555	7.12%	2.208%
4	4.586	556	574	606	rVB4	64190832	211036262	32.42%	10.053%
5	5.537	702	730	756	rBV4	92007890	457494461	70.27%	21.794%
6	8.854	1243	1274	1275	rBV6	150201520	651031541	100.00%	31.014%
7	10.238	1492	1501	1506	rBV	10829934	14145828	2.17%	0.674%
8	10.347	1512	1519	1525	rBV	32264497	43662928	6.71%	2.080%
9	10.689	1569	1575	1580	rBV	23753880	30537640	4.69%	1.455%
10	11.420	1690	1695	1703	rBV	15248292	27463627	4.22%	1.308%
11	11.494	1703	1707	1721	rVB	7412736	10181693	1.56%	0.485%
12	11.664	1721	1735	1736	rBV8	145736859	458656535	70.45%	21.850%
13	11.823	1753	1761	1765	rBV	24368711	35094059	5.39%	1.672%
14	11.878	1765	1770	1775	rVV	54474833	68369978	10.50%	3.257%
15	12.134	1808	1812	1818	rVB	8670598	10962387	1.68%	0.522%
16	13.816	2082	2088	2093	rBV	6908398	8475401	1.30%	0.404%

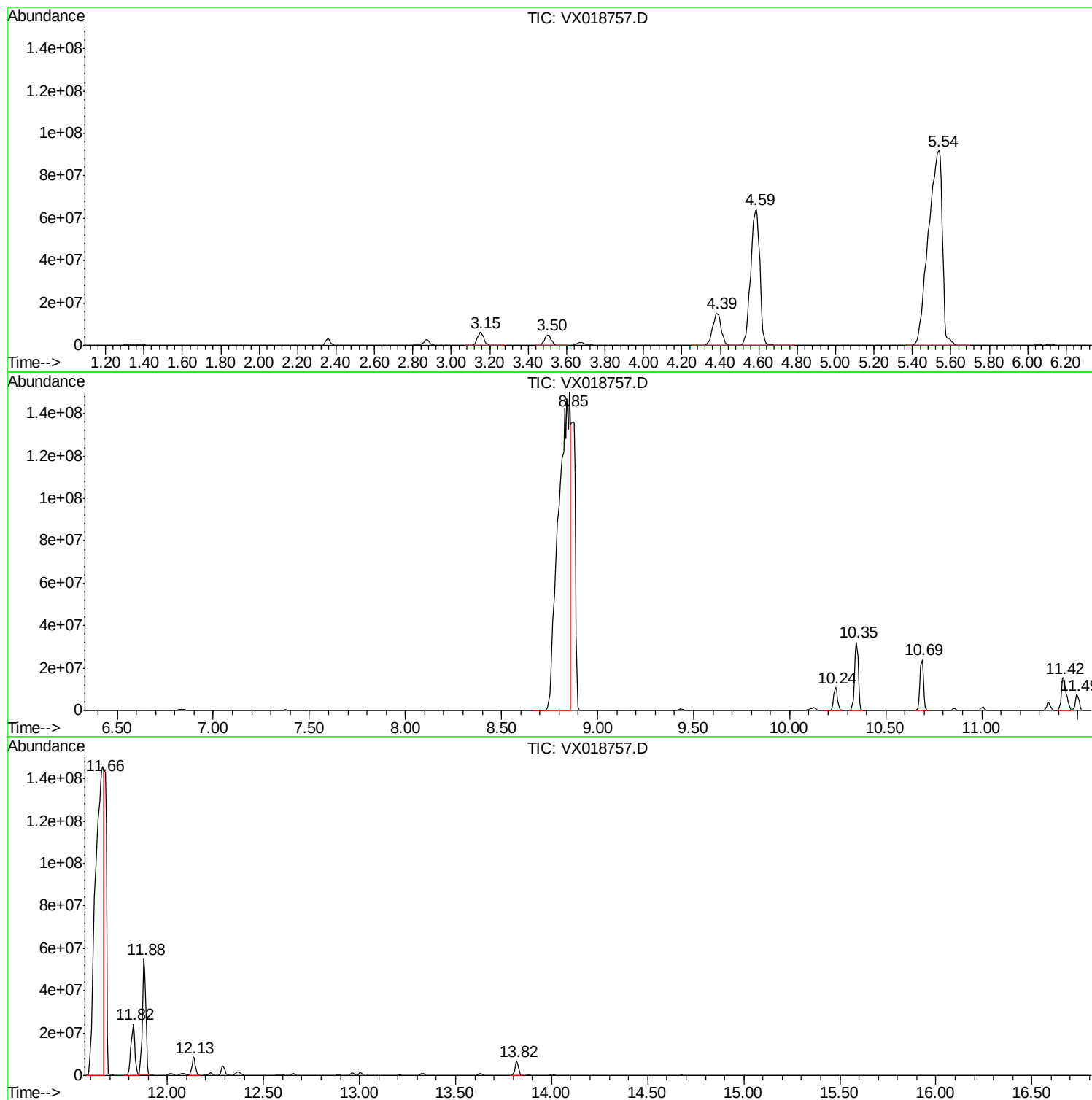
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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



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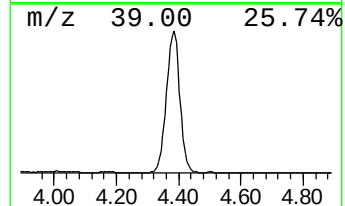
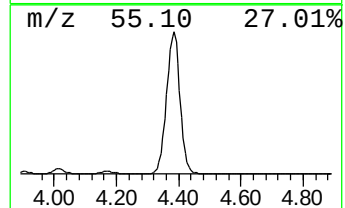
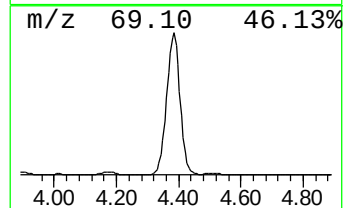
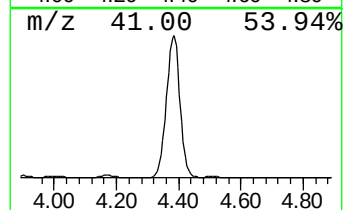
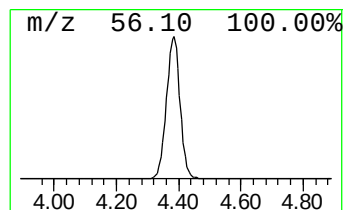
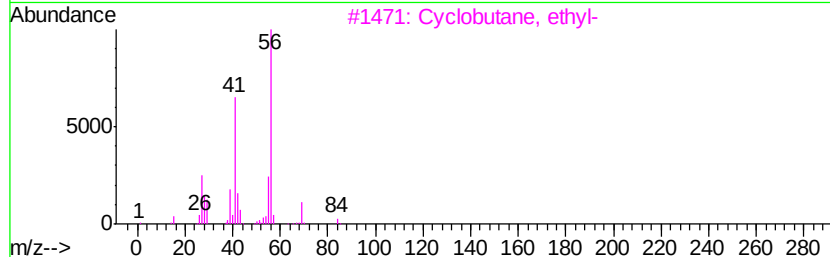
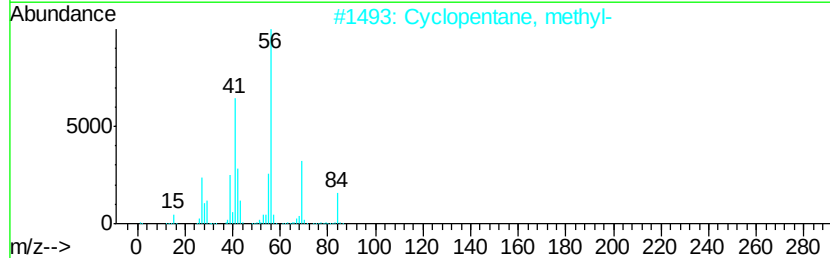
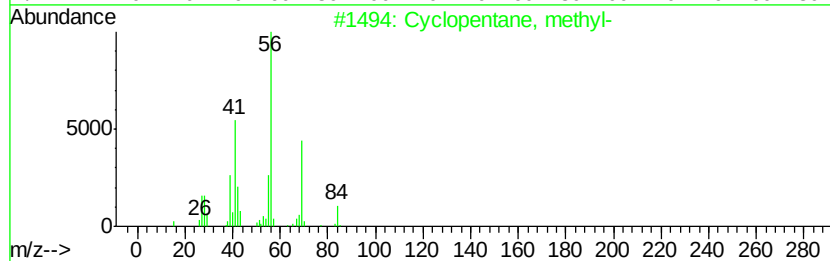
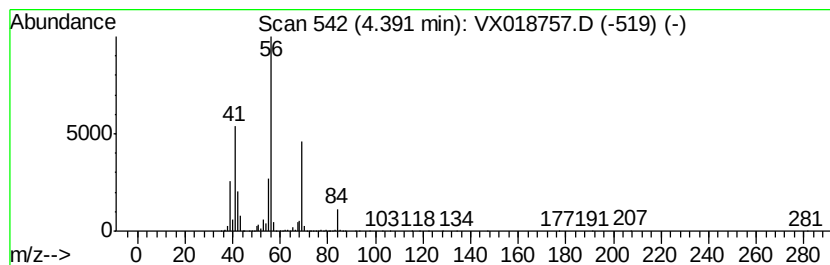
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Cyclic4.39 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.39	0.51 ug/L	46359600	1,4-Difluorobenzene	6.84	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	78
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72



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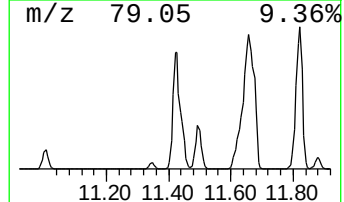
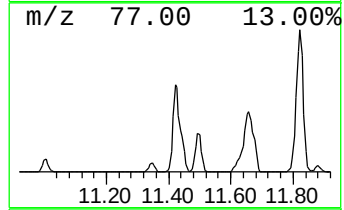
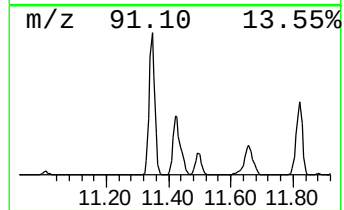
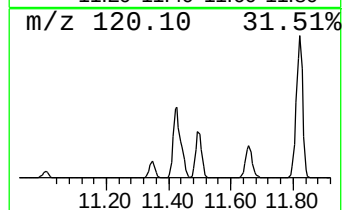
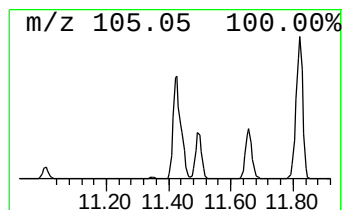
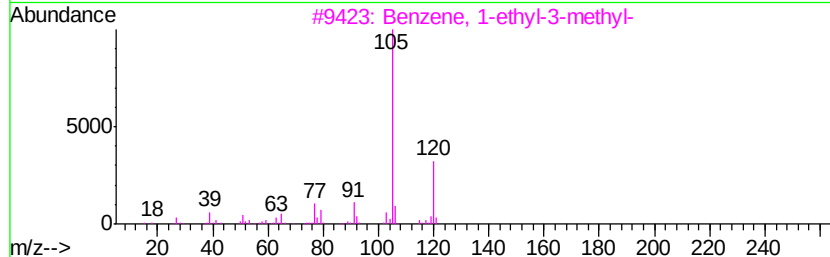
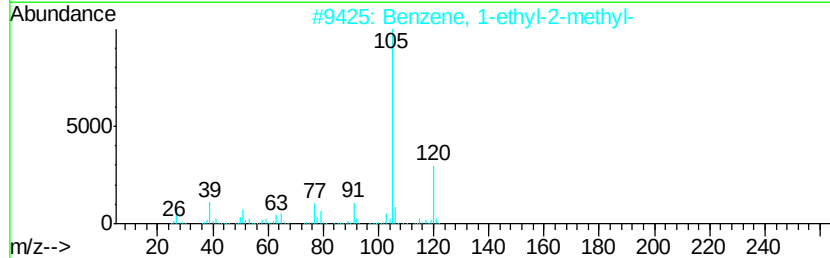
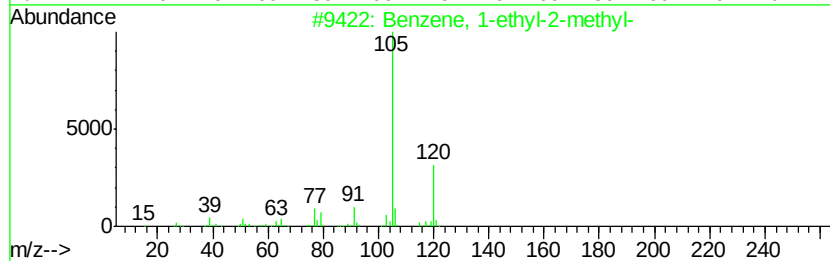
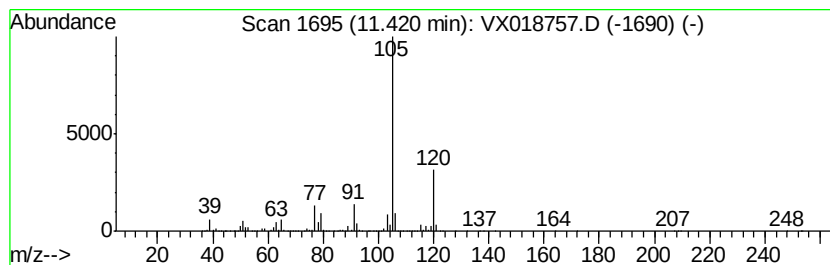
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	12.53 ug/L	27463600	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
4		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
5		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



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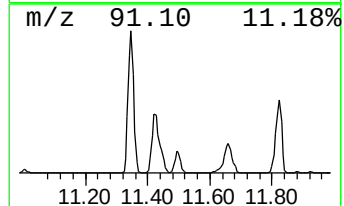
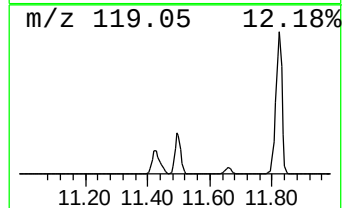
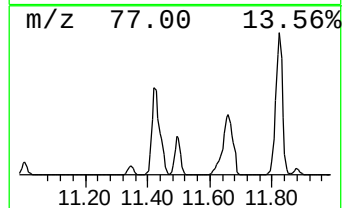
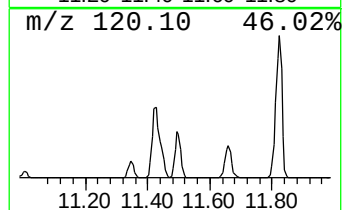
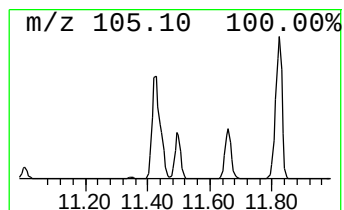
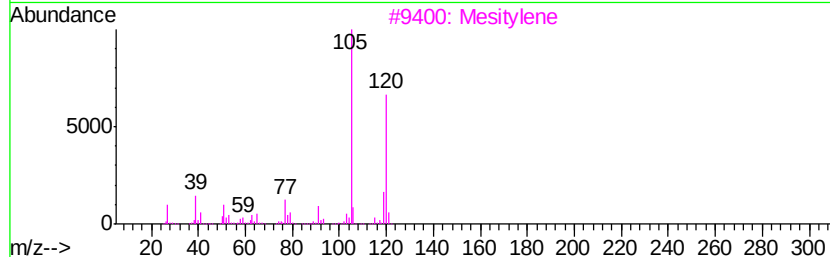
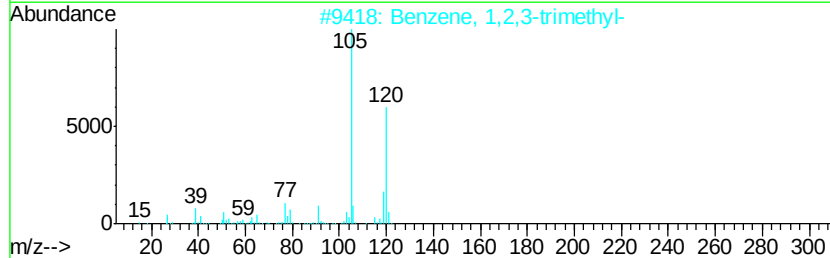
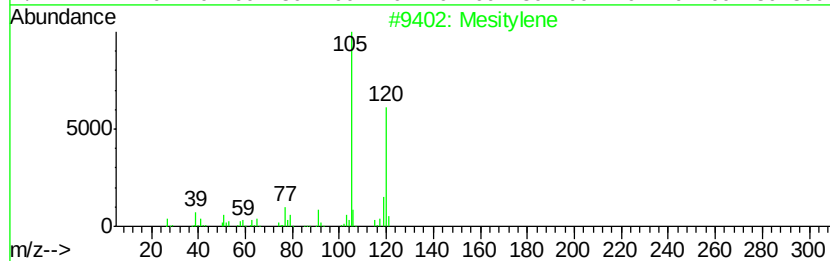
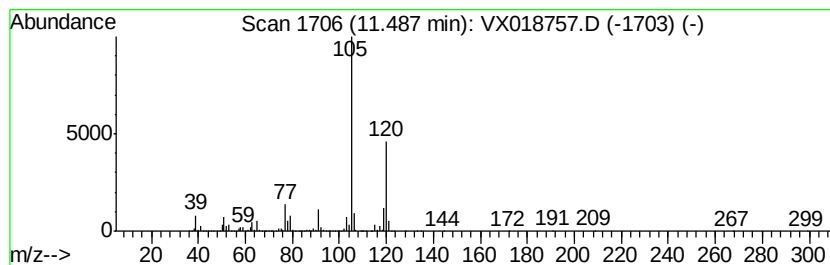
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Peak Number 3 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.49	4.64 ug/L	10181700	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene		120	C9H12	000108-67-8	97
2	Benzene, 1,2,3-trimethyl-		120	C9H12	000526-73-8	97
3	Mesitylene		120	C9H12	000108-67-8	95
4	Benzene, 1,2,4-trimethyl-		120	C9H12	000095-63-6	94
5	Mesitylene		120	C9H12	000108-67-8	94



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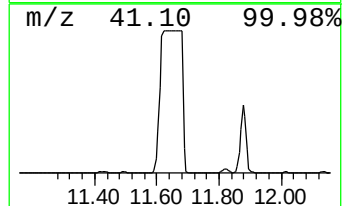
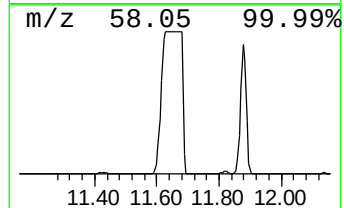
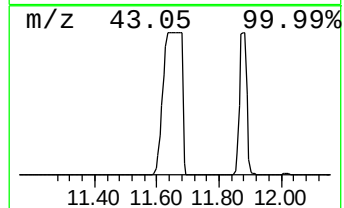
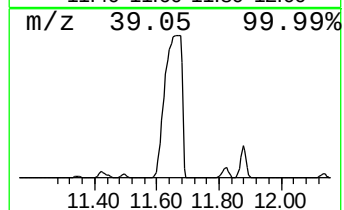
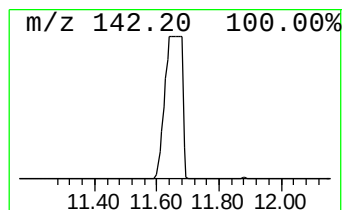
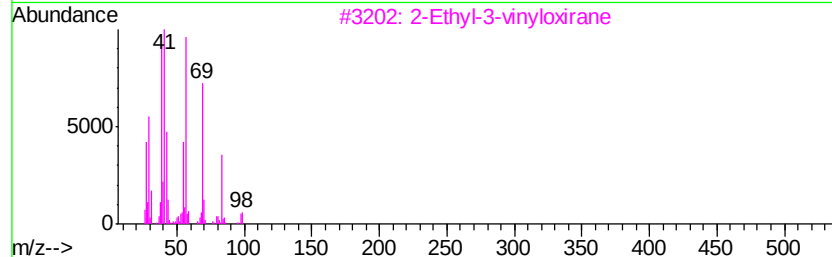
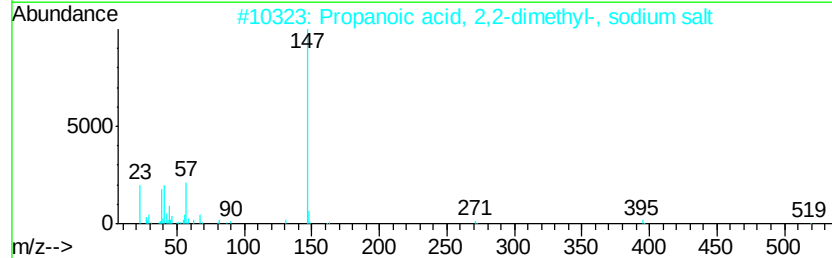
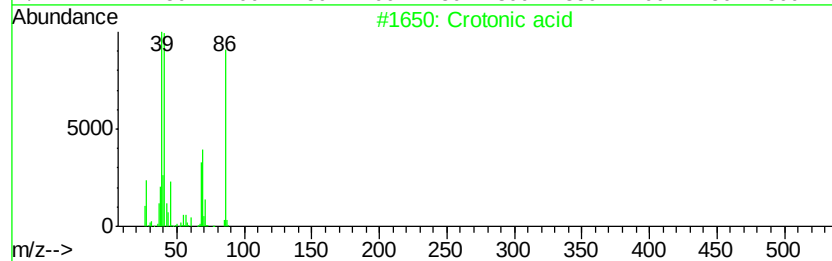
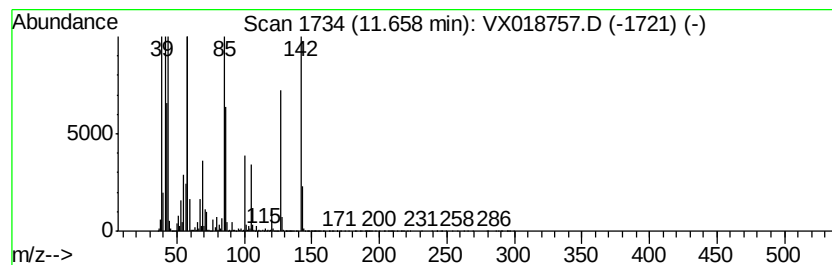
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	209.20 ug/L	458657000	1,4-Dichlorobenzene-d4	12.07

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Crotonic acid	86	C4H6O2	003724-65-0	35
2		Propanoic acid, 2,2-dimethyl-, s...	124	C5H9NaO2	001184-88-9	27
3		2-Ethyl-3-vinloxirane	98	C6H10O	034485-78-4	25
4		2-Butenoic acid, (E)-	86	C4H6O2	000107-93-7	25
5		4-Nonanone, 2,6,8-trimethyl-	184	C12H24O	000123-18-2	22



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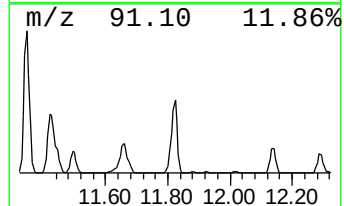
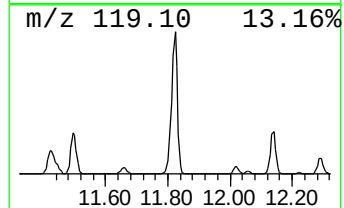
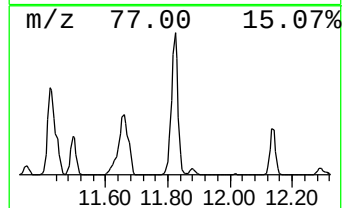
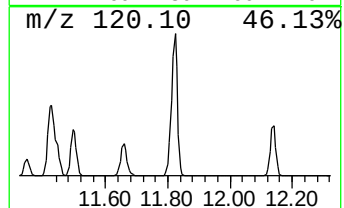
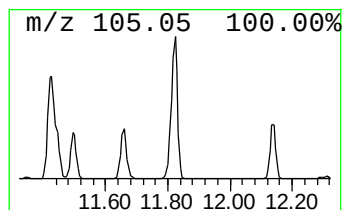
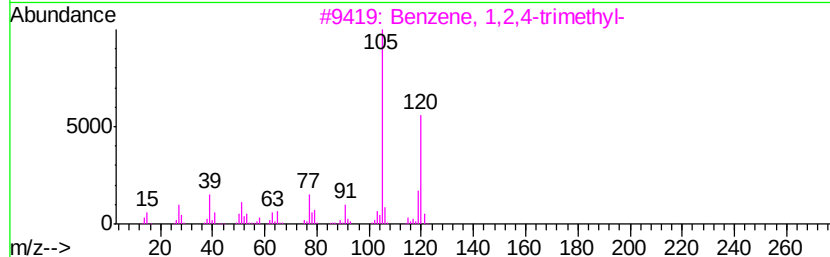
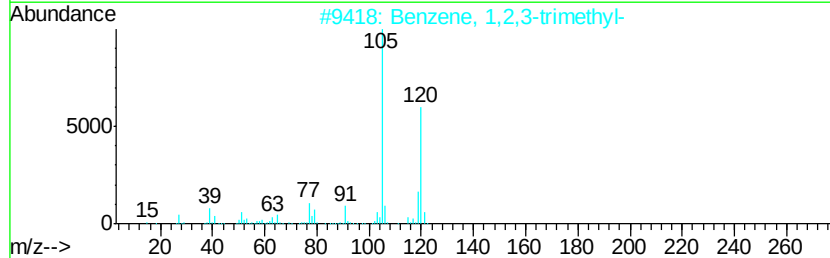
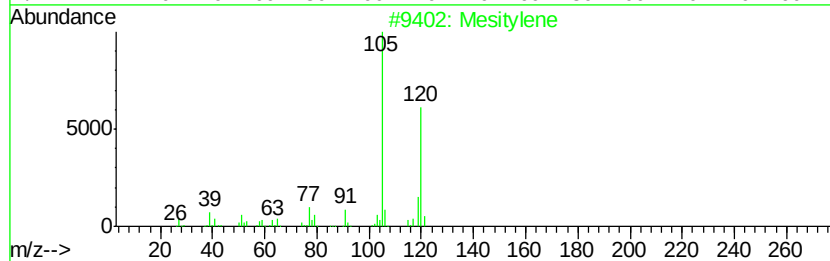
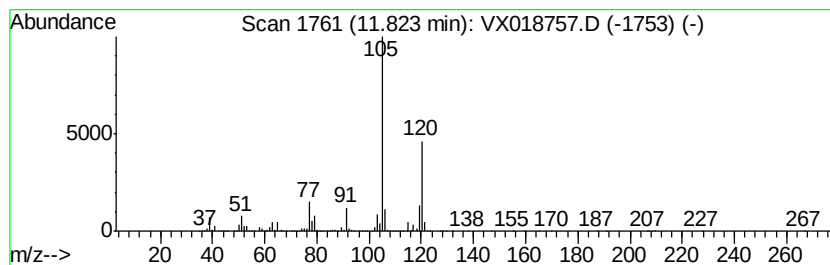
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Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	16.01 ug/L	35094100	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mesitylene	120	C9H12	000108-67-8	97
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	95
4		Mesitylene	120	C9H12	000108-67-8	94
5		Mesitylene	120	C9H12	000108-67-8	94



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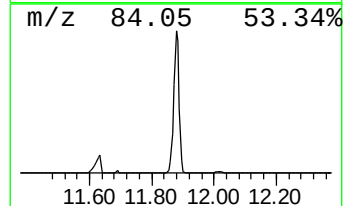
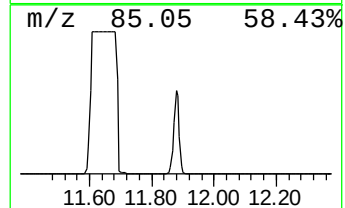
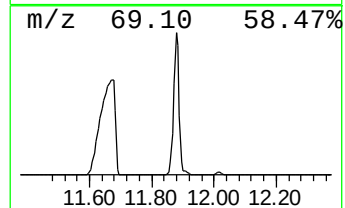
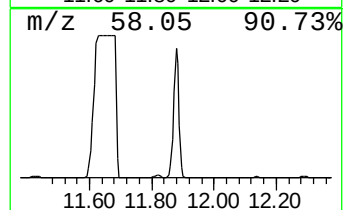
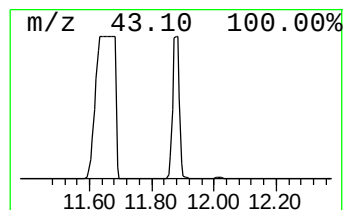
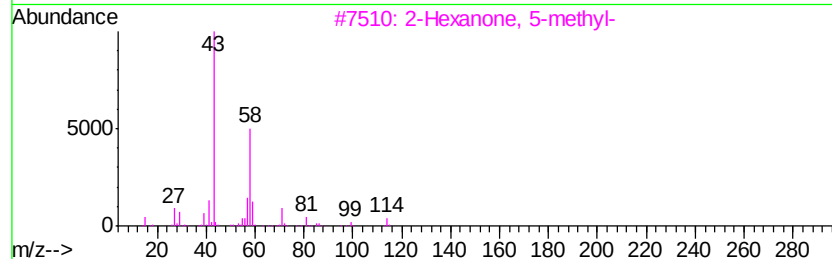
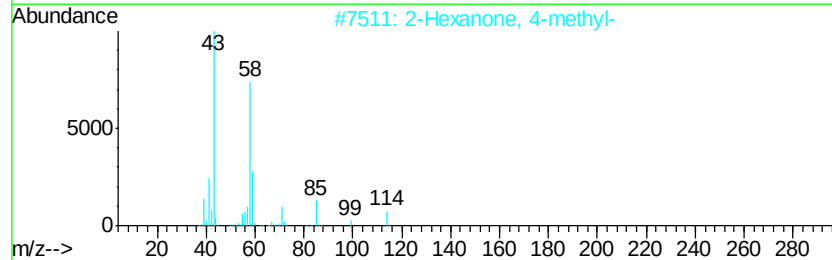
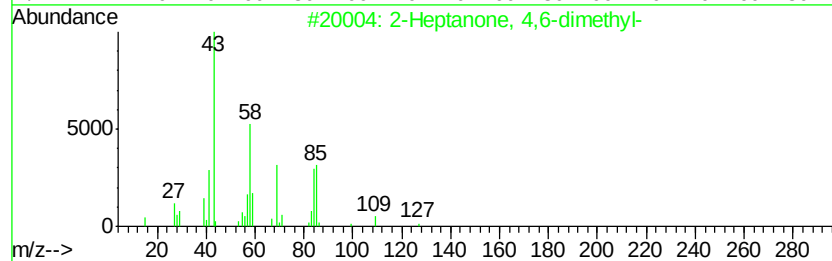
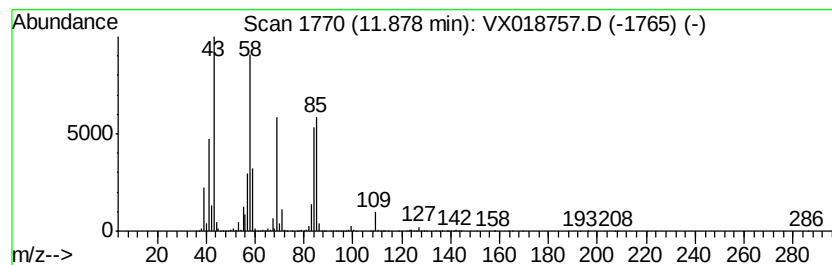
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TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Heptanone, 4,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.88	31.18 ug/L	68370000	1,4-Dichlorobenzene-d4	12.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Heptanone, 4,6-dimethyl-	142 C9H18O	019549-80-5	86
2	2-Hexanone, 4-methyl-	114 C7H14O	000105-42-0	43
3	2-Hexanone, 5-methyl-	114 C7H14O	000110-12-3	38
4	Nonane, 5-methyl-	142 C10H22	015869-85-9	35
5	Hexane, 3-ethyl-	114 C8H18	000619-99-8	35



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX100220\
Data File : VX018757.D
Acq On : 02 Oct 2020 19:05
Operator : JC/SP
Sample : L4239-04
Misc : 25.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3N3

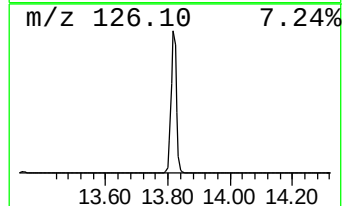
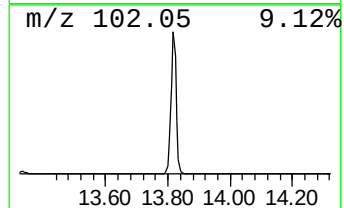
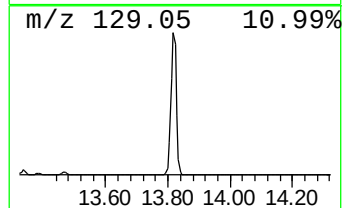
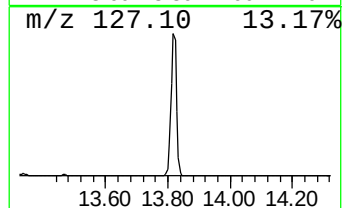
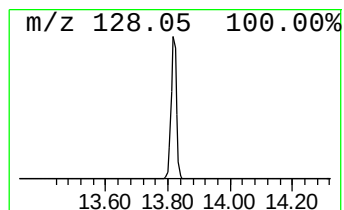
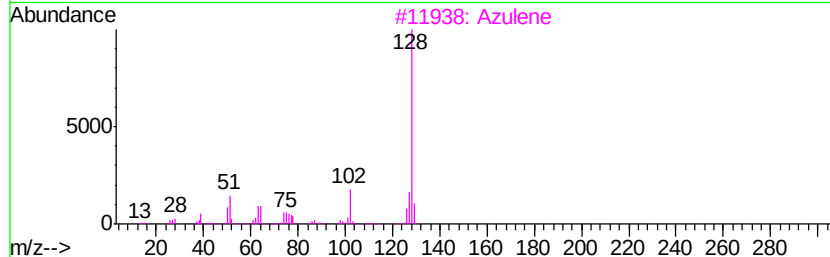
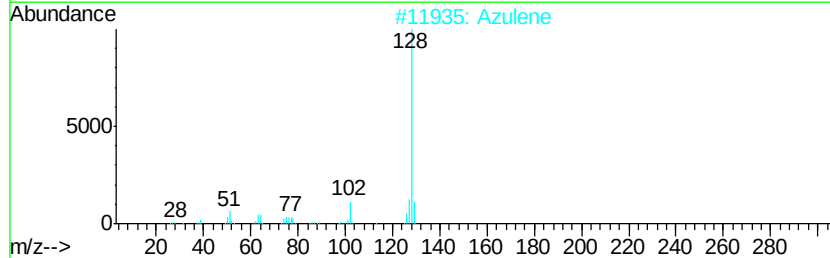
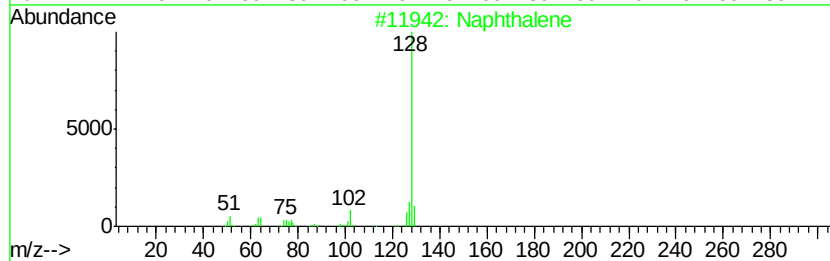
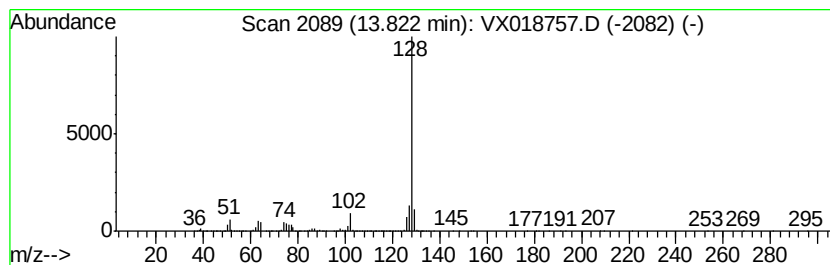
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Azulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	3.87 ug/L	8475400	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene	128	C10H8	000091-20-3	95
2		Azulene	128	C10H8	000275-51-4	94
3		Azulene	128	C10H8	000275-51-4	91
4		Azulene	128	C10H8	000275-51-4	91
5		Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100220\
Data File : VX018757.D
Acq On : 02 Oct 2020 19:05
Operator : JC/SP
Sample : L4239-04
Misc : 25.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BG3N3

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\SOMXTR100220WMA.M
Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	4.39	0.5	ug/L	46359600	1	6.84	457494000	5.0
Benzene, 1-ethyl-...	11.42	12.5	ug/L	27463600	3	12.07	10962400	5.0
Mesitylene	11.49	4.6	ug/L	10181700	3	12.07	10962400	5.0
unknown-01	11.66	209.2	ug/L	458657000	3	12.07	10962400	5.0
Benzene, 1,2,3-tr...	11.82	16.0	ug/L	35094100	3	12.07	10962400	5.0
2-Heptanone, 4,6-...	11.88	31.2	ug/L	68370000	3	12.07	10962400	5.0
Azulene	13.82	3.9	ug/L	8475400	3	12.07	10962400	5.0