

Data Path : W:\HPCHEM1\MSVOA V\DATA\VV051518\
 Data File : VV005916.D
 Acq On : 15 May 2018 15:29
 Operator : SY/MD
 Sample : J2905-04
 Misc : 25.0 mL/MSVOA V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : W:\HPCHEM1\MSVOA V\METHOD\SOMVTR050518WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

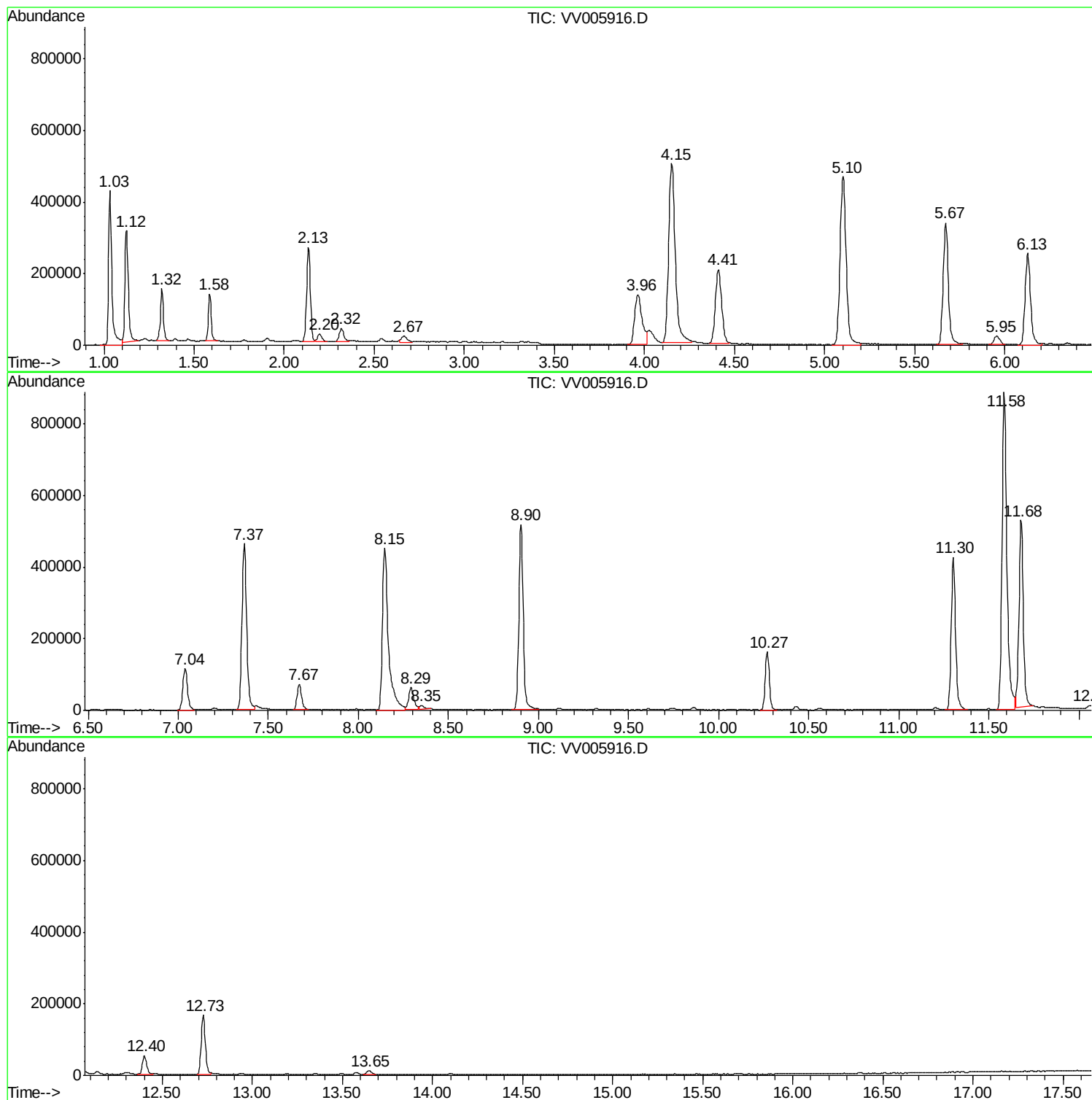
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.032	26	44	65	rBV	430904	537544	31.78%	3.989%
2	1.125	65	73	93	rVB	307936	404349	23.90%	3.001%
3	1.321	125	134	146	rVB	144157	164069	9.70%	1.218%
4	1.585	209	216	230	rVB	130854	150086	8.87%	1.114%
5	2.135	376	387	397	rBV	263257	374870	22.16%	2.782%
6	2.196	400	406	418	rVB	22158	34107	2.02%	0.253%
7	2.318	435	444	458	rBV	35756	61716	3.65%	0.458%
8	2.665	545	552	566	rVB3	16231	35390	2.09%	0.263%
9	3.961	937	955	971	rBV	139893	404040	23.89%	2.999%
10	4.151	998	1014	1049	rBV	499215	1275887	75.43%	9.469%
11	4.411	1079	1095	1113	rBV	204843	487049	28.79%	3.615%
12	5.102	1290	1310	1341	rBV2	469283	1101690	65.13%	8.176%
13	5.671	1471	1487	1516	rBV	341024	694079	41.03%	5.151%
14	5.954	1562	1575	1589	rBV6	23466	53196	3.14%	0.395%
15	6.128	1612	1629	1653	rBV	255909	535363	31.65%	3.973%
16	7.038	1898	1912	1928	rBV	115206	210183	12.43%	1.560%
17	7.366	2000	2014	2032	rBV	463705	841925	49.77%	6.248%
18	7.671	2098	2109	2124	rBV2	72209	123708	7.31%	0.918%
19	8.147	2242	2257	2292	rBV3	451127	1047147	61.91%	7.772%
20	8.292	2292	2302	2314	rVV2	60870	118548	7.01%	0.880%
21	8.353	2316	2321	2335	rVB2	9535	17254	1.02%	0.128%
22	8.903	2476	2492	2523	rBV	517732	870124	51.44%	6.458%
23	10.269	2904	2917	2934	rBV	162478	257164	15.20%	1.909%
24	11.301	3224	3238	3263	rBV	425820	715223	42.28%	5.308%
25	11.584	3312	3326	3345	rBV	886490	1691533	100.00%	12.554%
26	11.678	3346	3355	3375	rVB	519439	878766	51.95%	6.522%
27	12.063	3462	3475	3488	rBV	8803	20218	1.20%	0.150%
28	12.401	3567	3580	3595	rBV3	52565	86463	5.11%	0.642%
29	12.726	3670	3681	3695	rBV	165566	263277	15.56%	1.954%
30	13.645	3957	3967	3979	rBV6	10438	19146	1.13%	0.142%

Sum of corrected areas: 13474114

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Quant Title : TRACE VOA SOM01.0

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



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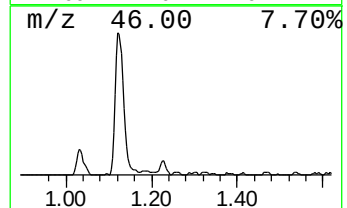
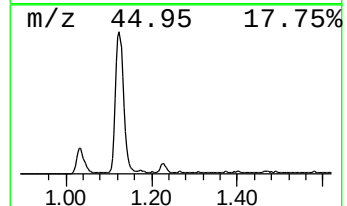
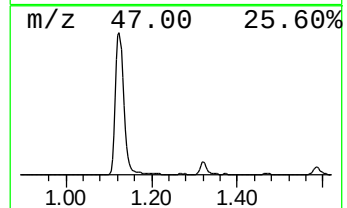
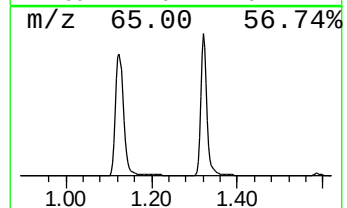
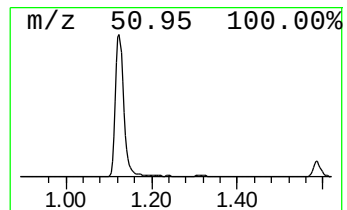
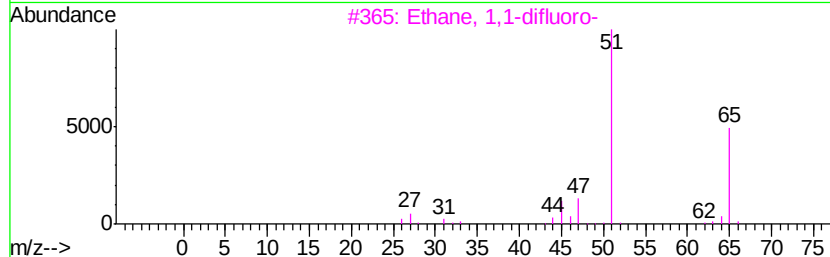
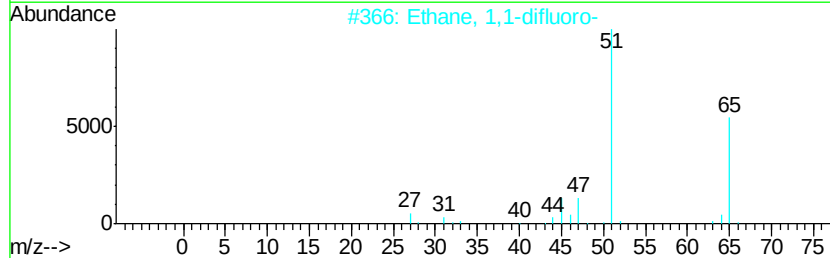
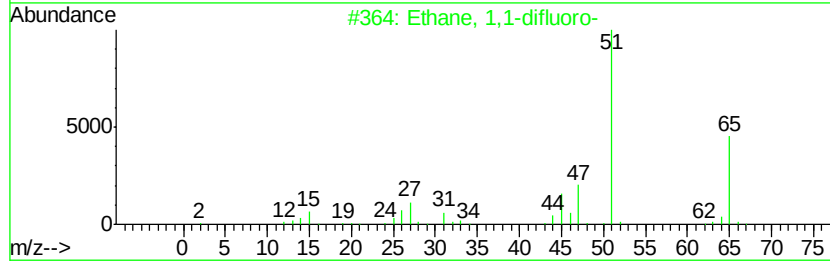
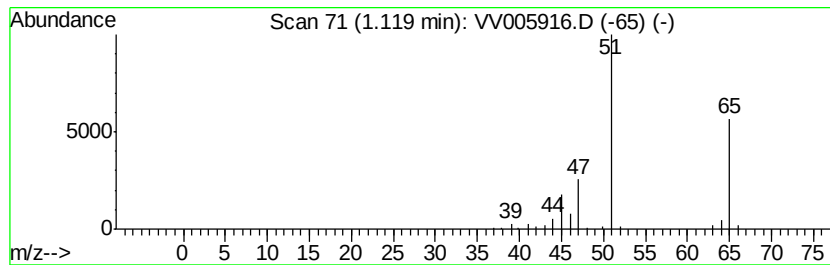
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethane, 1,1-difluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.12	2.91 ug/L	404349	1,4-Difluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
2			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
3			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
4			Propiolonitrile	51	C3HN	001070-71-9	3
5			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2



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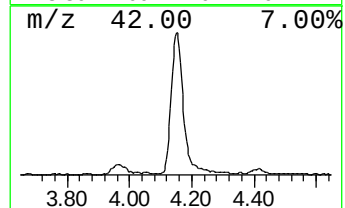
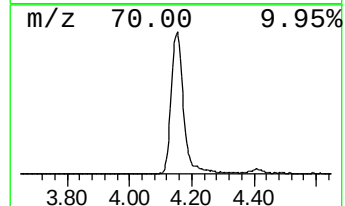
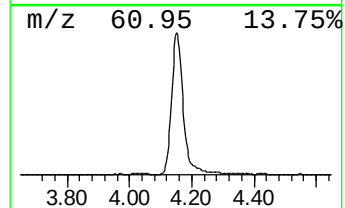
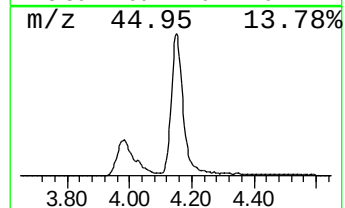
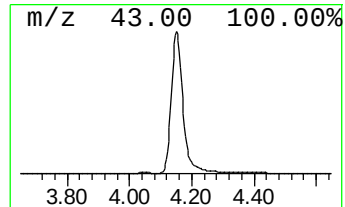
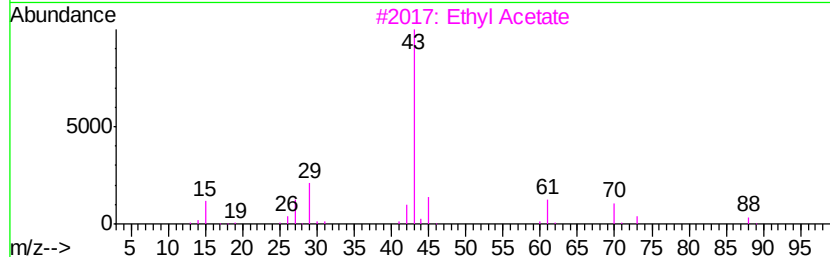
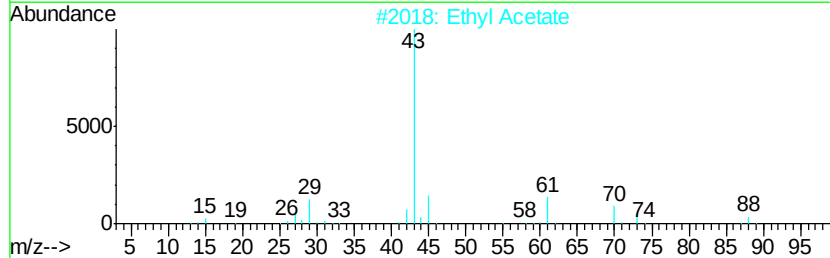
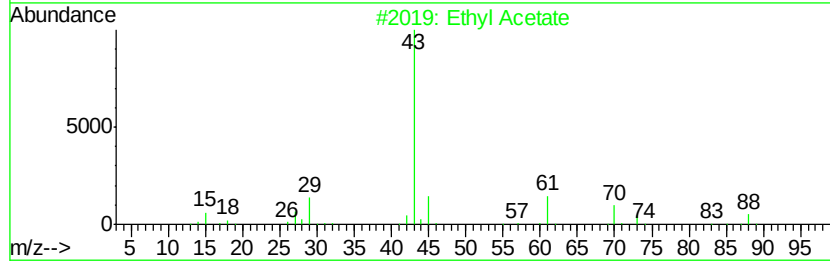
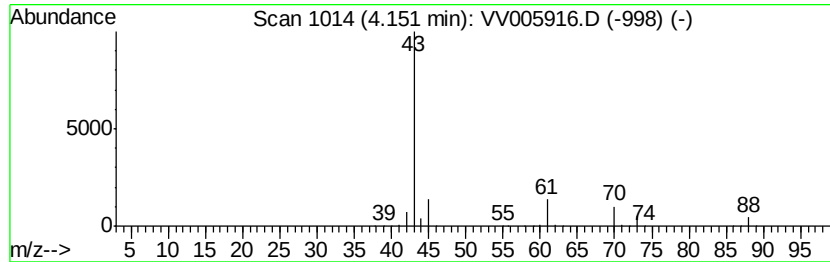
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.15	9.19 ug/L	1275890	1,4-Difluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	90
2		Ethyl Acetate	88	C4H8O2	000141-78-6	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	9
5		(3-Methyl-oxiran-2-yl)-methanol	88	C4H8O2	1000194-22-9	9



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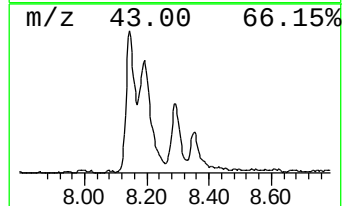
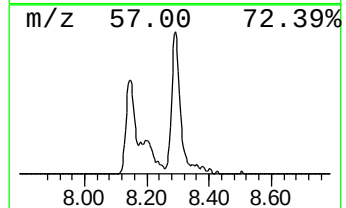
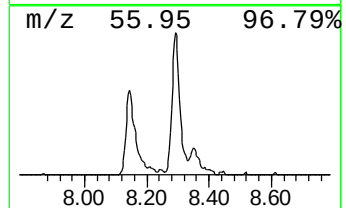
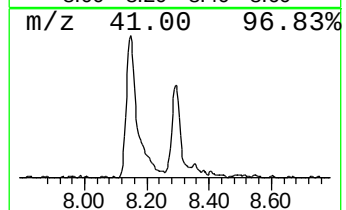
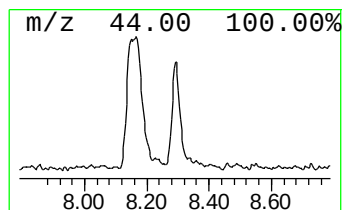
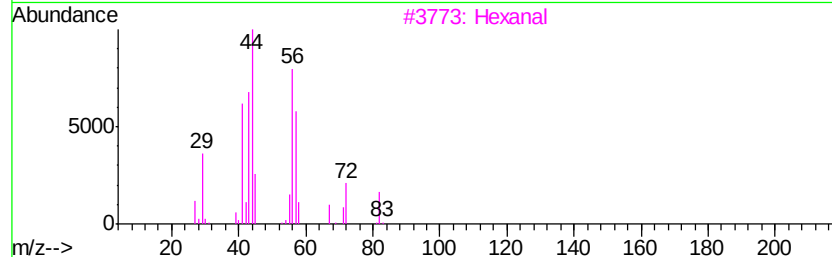
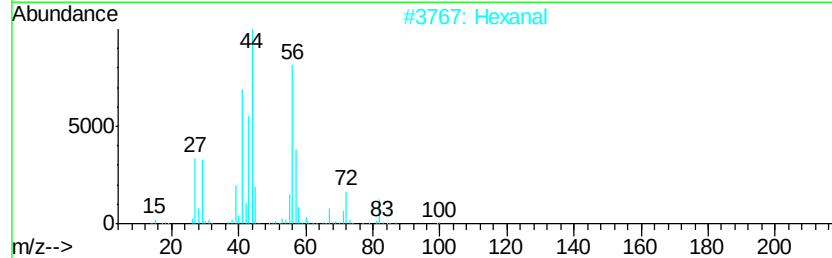
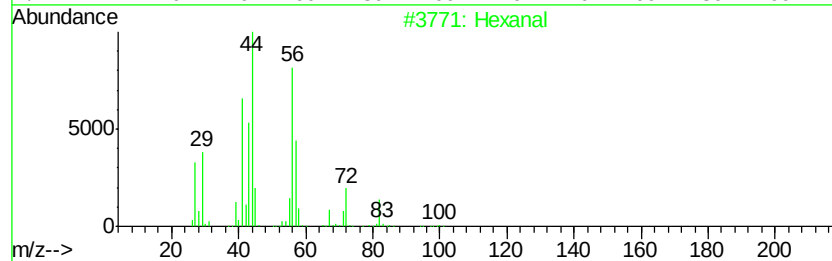
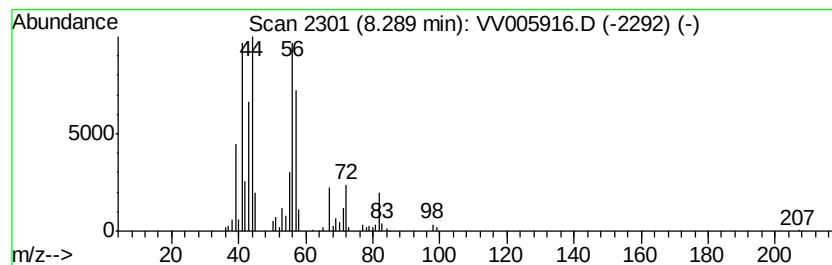
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Hexanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.29	0.68 ug/L	118548	Chlorobenzene-d5	8.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	81
2		Hexanal	100	C6H12O	000066-25-1	64
3		Hexanal	100	C6H12O	000066-25-1	64
4		Hexanal	100	C6H12O	000066-25-1	53
5		Butanal, 3-methyl-	86	C5H10O	000590-86-3	38



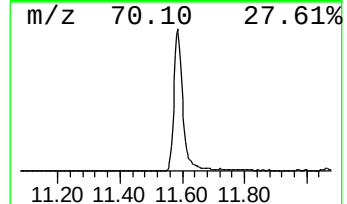
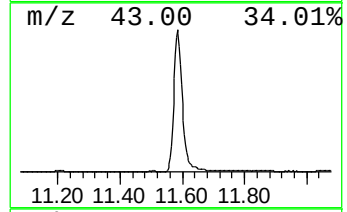
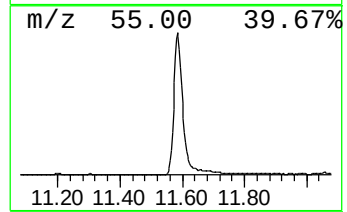
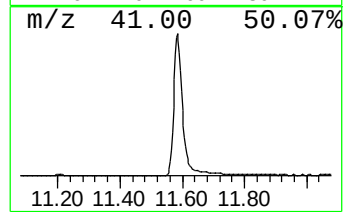
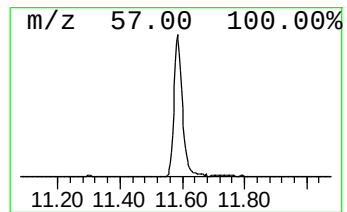
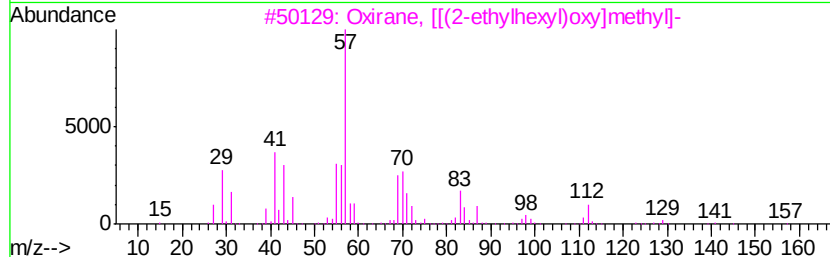
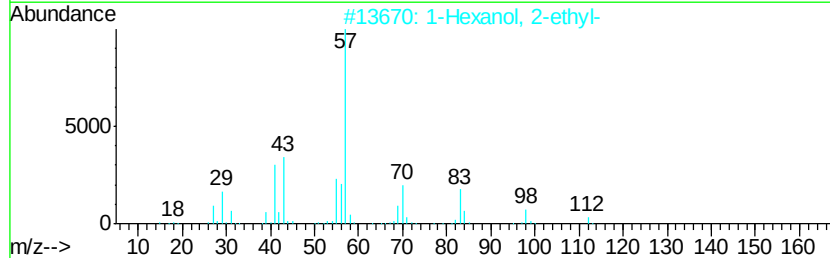
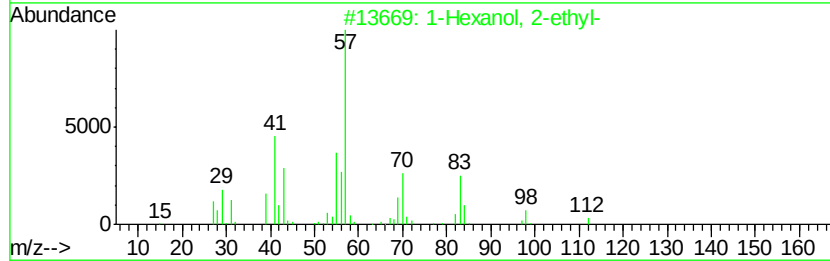
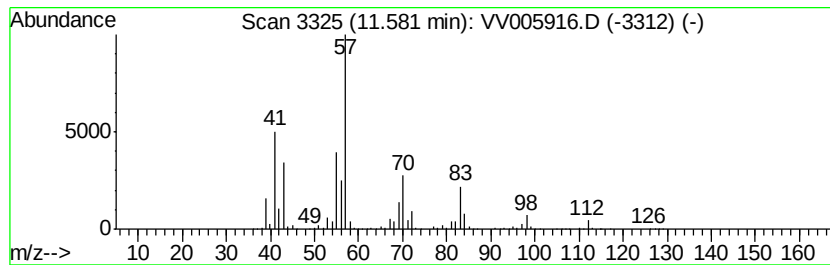
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Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.58	11.83 ug/L	1691530	1,4-Dichlorobenzene-d4	11.30	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	80
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3	Oxirane, [[(2-ethylhexyl)oxylmet...	186	C11H22O2	002461-15-6	64
4	Oxirane, [[(2-ethylhexyl)oxylmet...	186	C11H22O2	002461-15-6	59
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59



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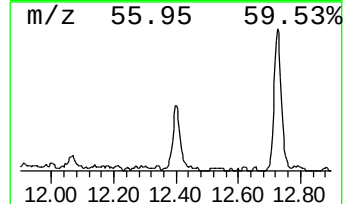
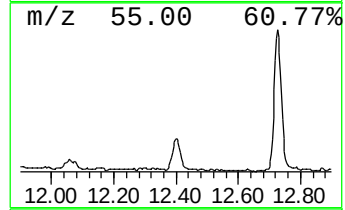
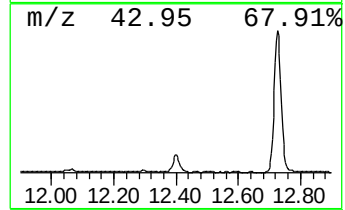
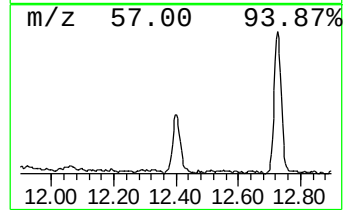
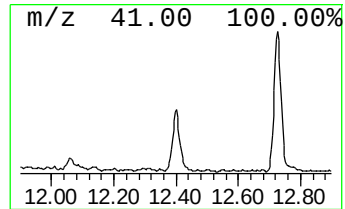
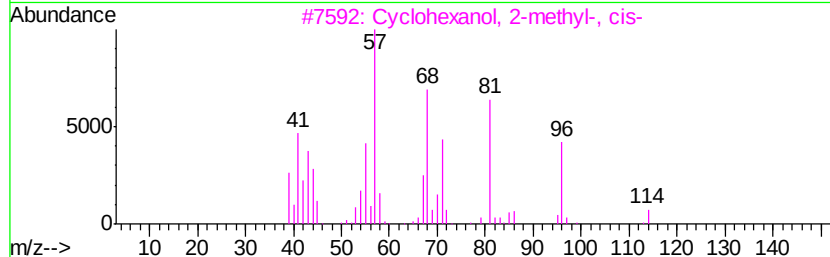
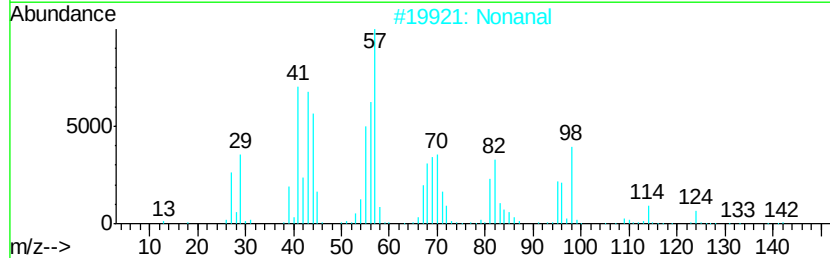
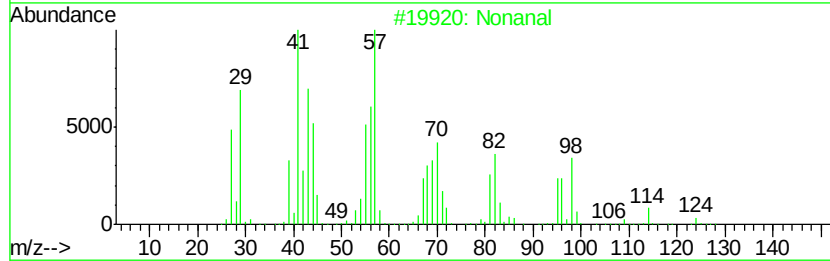
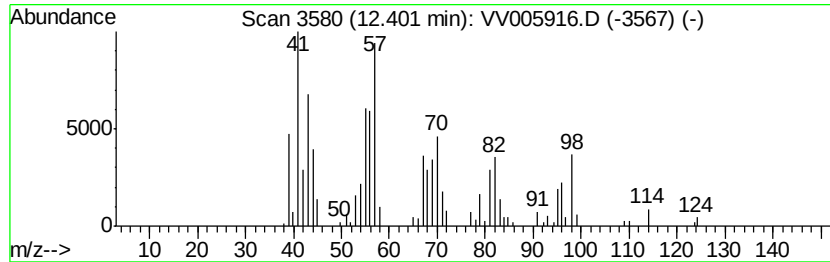
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Nonanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	0.60 ug/L	86463	1,4-Dichlorobenzene-d4	11.30

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	91
2	Nonanal		142	C9H18O	000124-19-6	58
3	Cyclohexanol, 2-methyl-, cis-		114	C7H14O	007443-70-1	42
4	Cyclohexanol, 4-methyl-		114	C7H14O	000589-91-3	38
5	Cyclohexanol, 2-methyl-, trans-		114	C7H14O	007443-52-9	38



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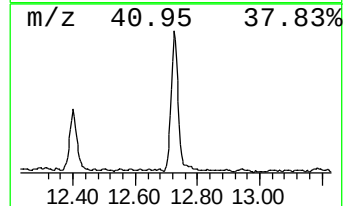
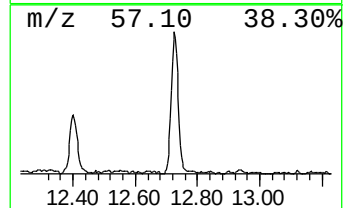
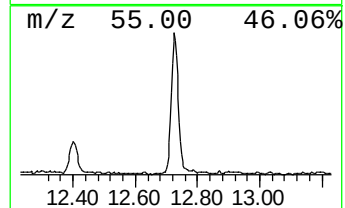
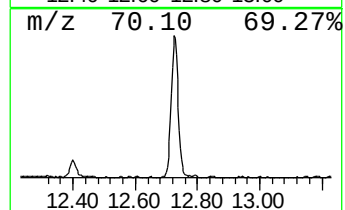
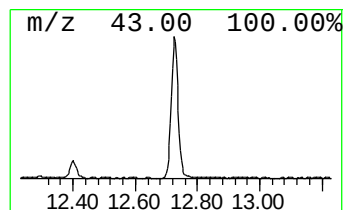
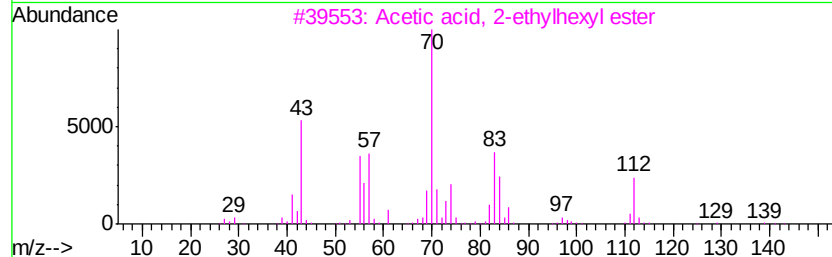
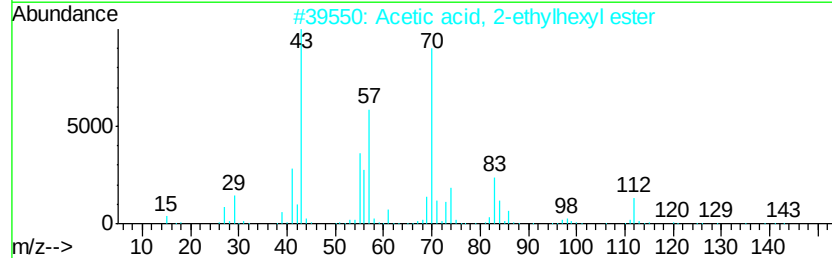
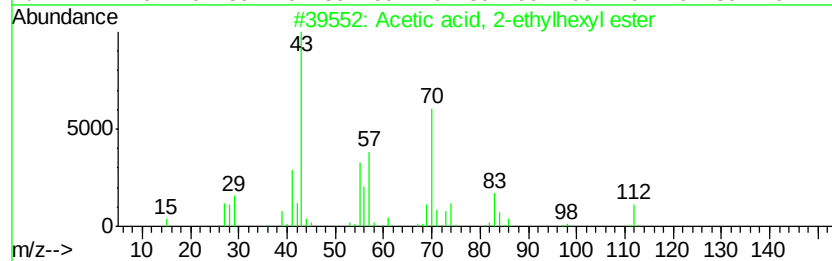
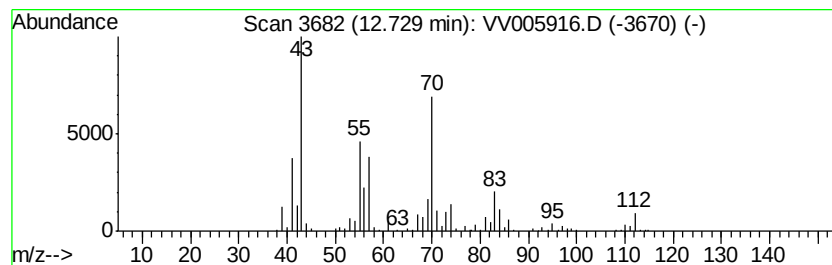
Quant Method : W:\HPCHEM1\MSVOA V\METHOD\SOMVTR050518WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Acetic acid, 2-ethylhexyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	1.84 ug/L	263277	1,4-Dichlorobenzene-d4	11.30

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	90
2		Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	90
3		Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	72
4		Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	70
5		3-Methylheptyl acetate	172	C10H20O2	072218-58-7	53



Data Path : W:\HPCHEM1\MSVOA_V\DATA\VV051518\
Data File : VV005916.D
Acq On : 15 May 2018 15:29
Operator : SY/MD
Sample : J2905-04
Misc : 25.0 mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_V\METHOD\SOMVTR050518WMA.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
Ethane, 1,1-diflu...	1.12	2.9	ug/L	404349	1	5.67	694079	5.0
Ethyl Acetate	4.15	9.2	ug/L	1275890	1	5.67	694079	5.0
Hexanal	8.29	0.7	ug/L	118548	2	8.90	870124	5.0
1-Hexanol, 2-ethyl-	11.58	11.8	ug/L	1691530	3	11.30	715223	5.0
Nonanal	12.40	0.6	ug/L	86463	3	11.30	715223	5.0
Acetic acid, 2-et...	12.73	1.8	ug/L	263277	3	11.30	715223	5.0