

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
 Data File : VU042152.D
 Acq On : 21 Jan 2021 15:46
 Operator : SY/MD
 Sample : M1170-12DL 4X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFT93DL

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_U\METHOD\SOMUTR012021WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC: VU042152.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	18	rVB2	12174	11938	2.33%	0.274%
2	1.600	72	81	91	rVB	51627	57704	11.28%	1.322%
3	1.735	117	123	132	rVB2	9575	12123	2.37%	0.278%
4	1.919	171	180	190	rVB	39107	49625	9.70%	1.137%
5	2.571	369	383	397	rBV	88664	147593	28.84%	3.381%
6	2.655	400	409	426	rVB2	4576	11737	2.29%	0.269%
7	3.057	525	534	544	rVB2	3029	5396	1.05%	0.124%
8	3.195	565	577	587	rBV3	2670	5978	1.17%	0.137%
9	4.459	957	970	982	rBV4	2757	6956	1.36%	0.159%
10	4.642	1010	1027	1075	rBV	73554	239216	46.75%	5.481%
11	5.073	1143	1161	1178	rBV	78898	173426	33.89%	3.973%
12	5.732	1346	1366	1391	rBV2	153425	404753	79.10%	9.273%
13	6.256	1514	1529	1548	rBV	138536	260909	50.99%	5.978%
14	6.549	1595	1620	1638	rBV	152857	292547	57.17%	6.702%
15	6.700	1653	1667	1681	rBV	98480	188252	36.79%	4.313%
16	6.890	1713	1726	1736	rBV	5741	11800	2.31%	0.270%
17	7.574	1927	1939	1958	rBV	58531	102515	20.03%	2.349%
18	7.906	2029	2042	2056	rBV	190718	330173	64.52%	7.564%
19	7.976	2056	2064	2074	rVB2	6496	11007	2.15%	0.252%
20	8.185	2116	2129	2142	rBV	38089	65487	12.80%	1.500%
21	8.642	2258	2271	2306	rBV	280175	511700	100.00%	11.723%
22	8.793	2306	2318	2341	rVB	33087	57045	11.15%	1.307%
23	9.423	2502	2514	2537	rBV	189284	318403	62.22%	7.295%
24	9.770	2613	2622	2634	rVB3	5955	11598	2.27%	0.266%
25	10.140	2725	2737	2746	rVB3	3777	6425	1.26%	0.147%
26	10.352	2794	2803	2816	rBV3	13795	21618	4.22%	0.495%
27	10.764	2919	2931	2945	rBV	77145	123253	24.09%	2.824%
28	11.053	3011	3021	3031	rVB3	8063	13725	2.68%	0.314%
29	11.696	3211	3221	3232	rBV2	23038	35402	6.92%	0.811%
30	11.819	3244	3259	3274	rBV	203908	322313	62.99%	7.384%
31	12.069	3325	3337	3361	rBV2	40731	81976	16.02%	1.878%
32	12.201	3366	3378	3399	rVB	188395	308011	60.19%	7.057%
33	12.896	3581	3594	3608	rBV2	57637	87792	17.16%	2.011%
34	13.217	3684	3694	3706	rBV	52201	76450	14.94%	1.751%

Sum of corrected areas: 4364846

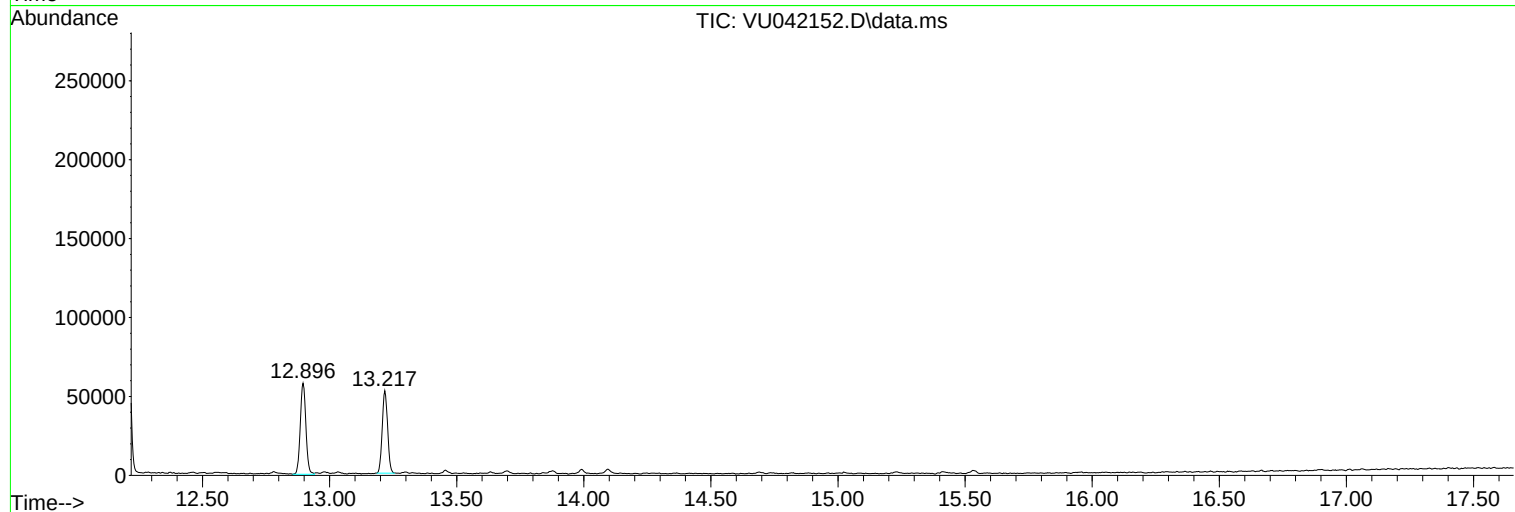
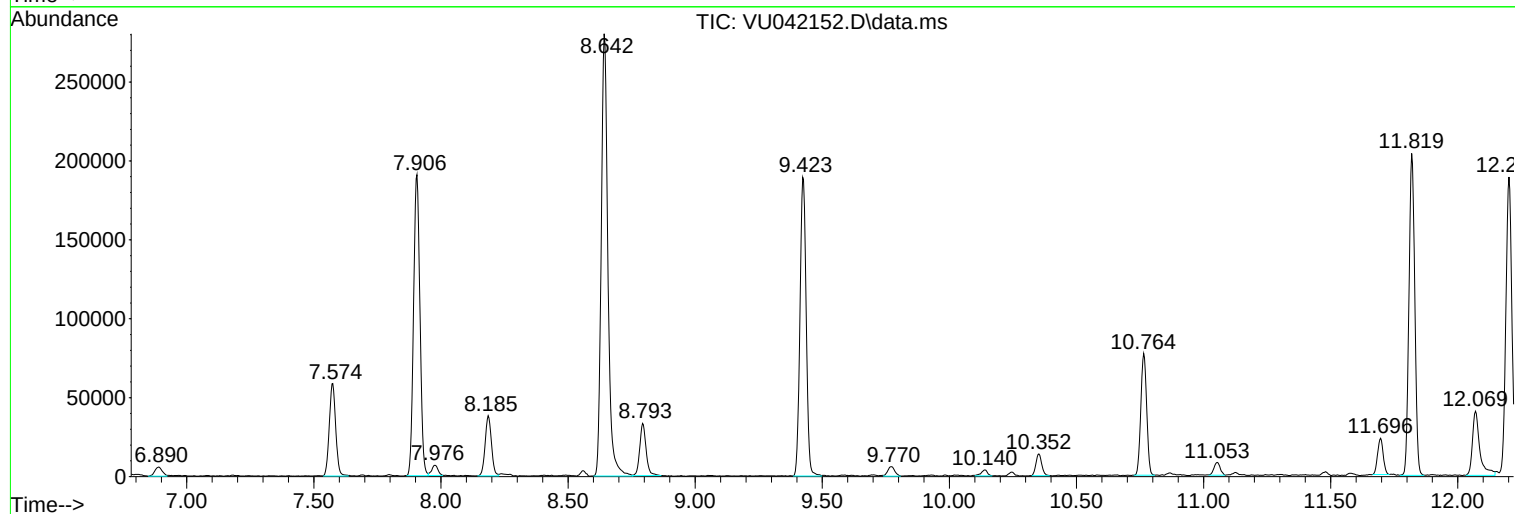
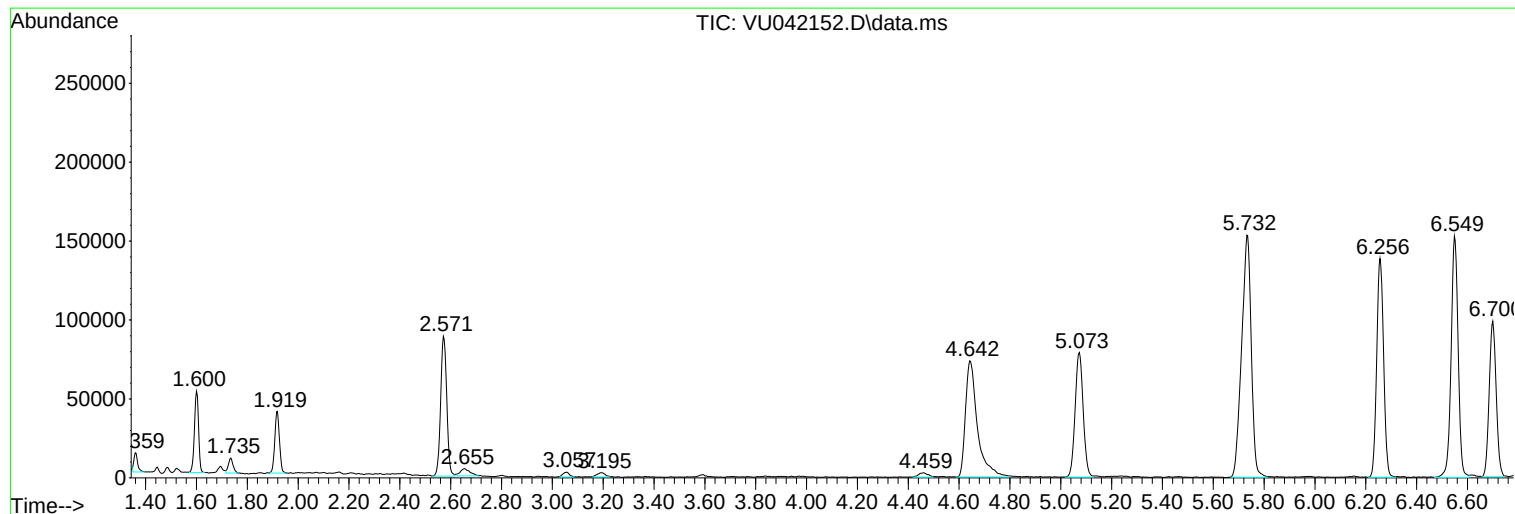
Instrument :
MSVOA_U
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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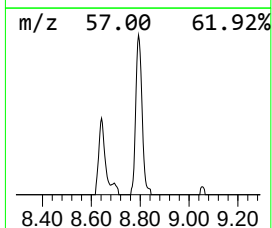
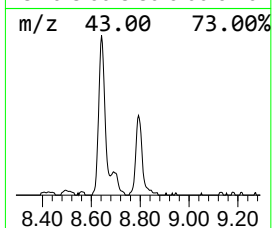
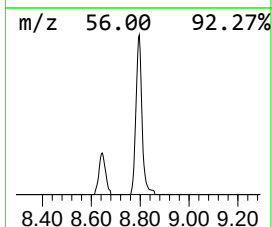
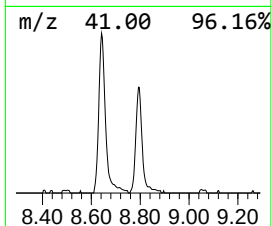
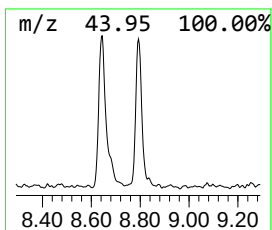
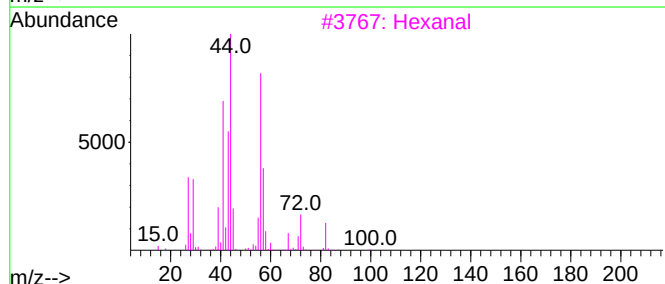
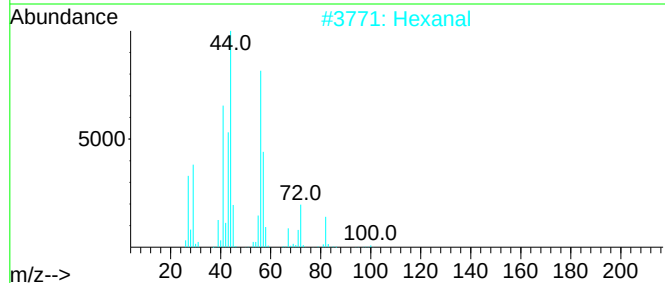
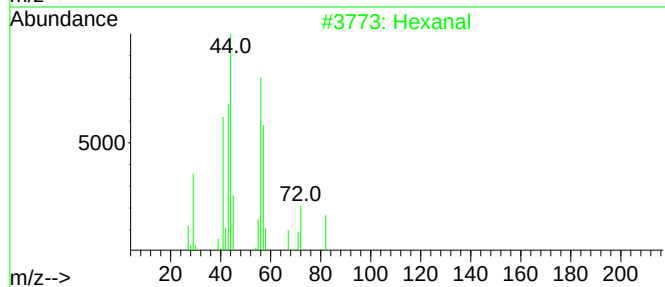
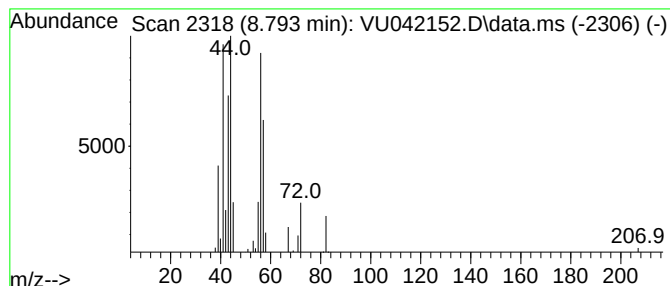
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.793	0.90 ug/L	57045	Chlorobenzene-d5	9.426

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	72
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	53
5	Butanal			72	C4H8O	000123-72-8	43



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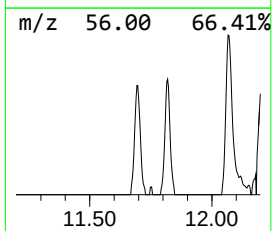
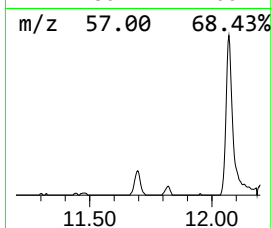
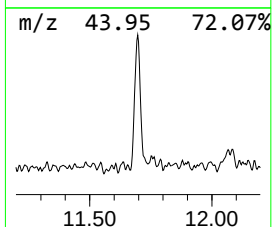
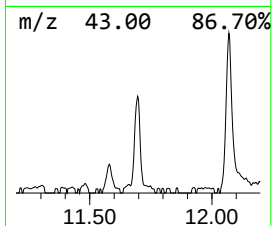
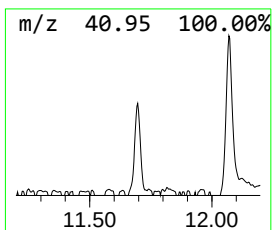
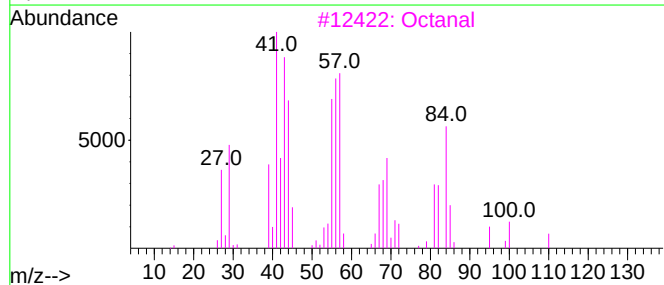
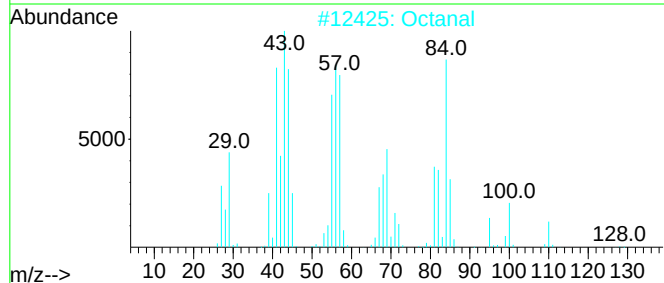
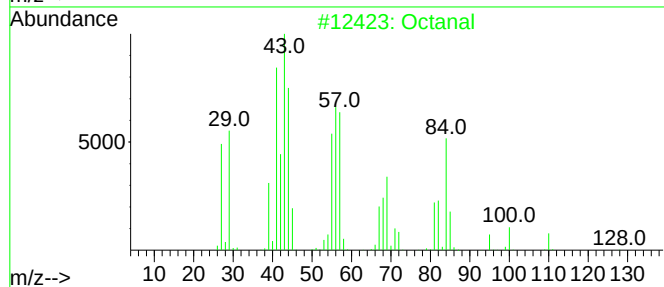
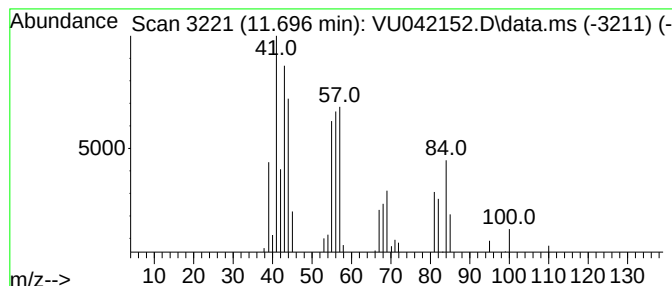
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Octanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.697	0.55 ug/L	35402	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	91
2	Octanal			128	C8H16O	000124-13-0	87
3	Octanal			128	C8H16O	000124-13-0	87
4	Octanal			128	C8H16O	000124-13-0	80
5	Octanal			128	C8H16O	000124-13-0	50



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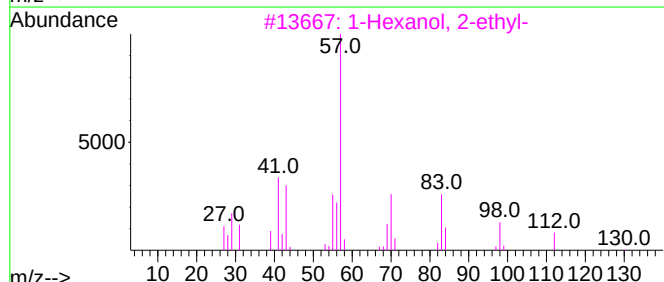
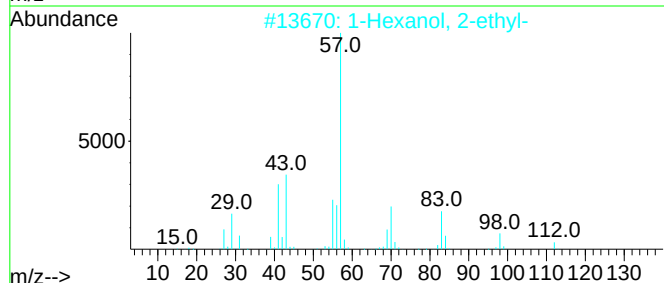
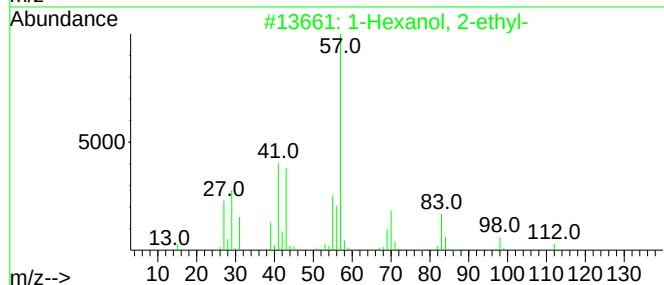
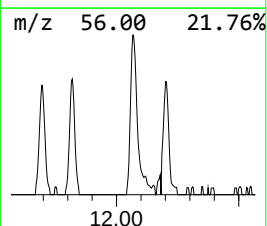
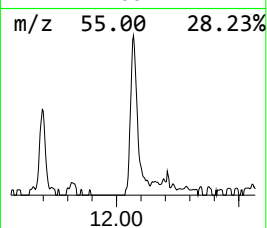
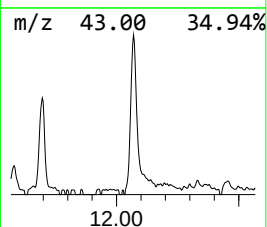
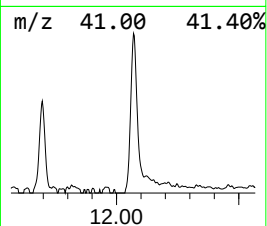
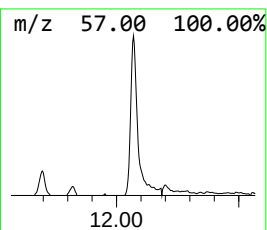
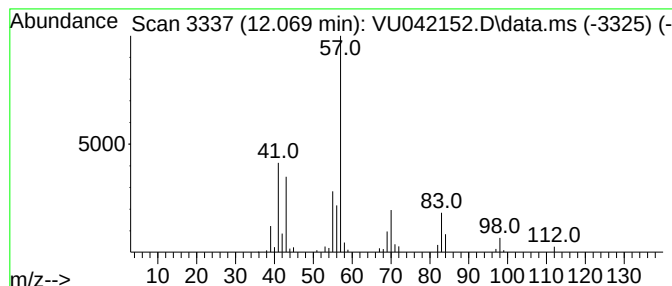
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.069	1.27 ug/L	81976	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64



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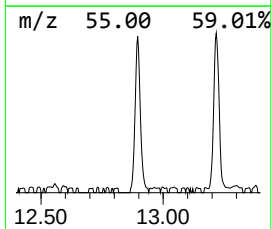
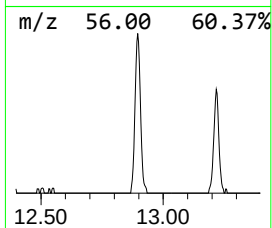
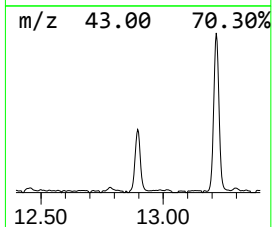
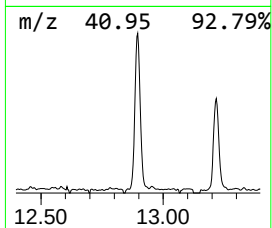
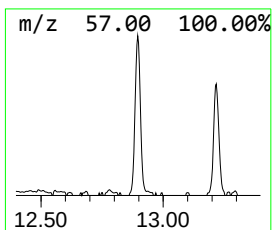
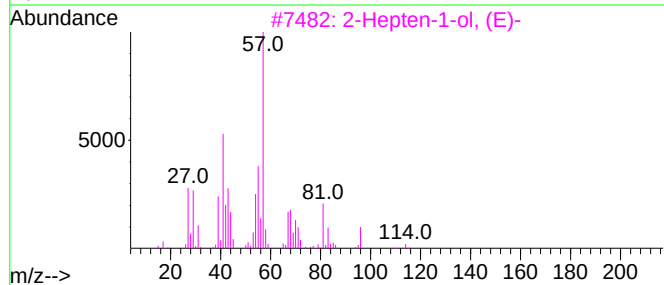
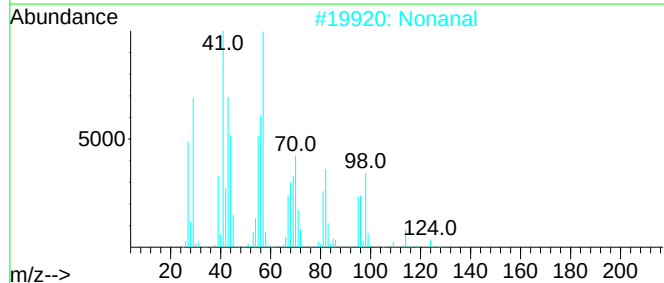
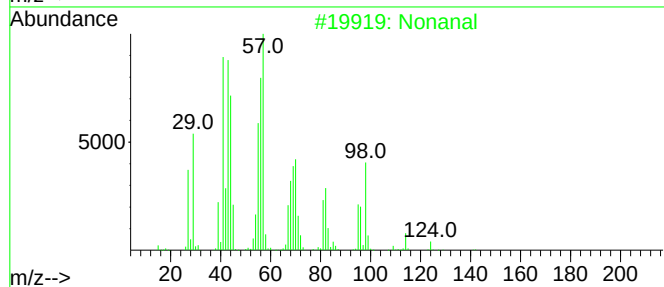
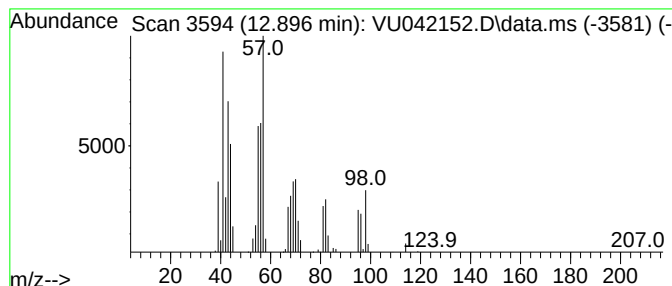
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.896	1.36 ug/L	87792	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	86
2			Nonanal	142	C9H18O	000124-19-6	59
3			2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	38
4			Butane, 1-isocyanato-	99	C5H9NO	000111-36-4	25
5			(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	22



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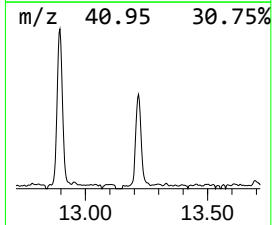
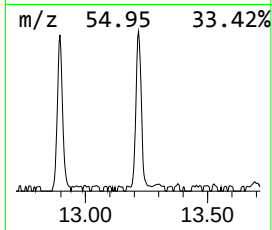
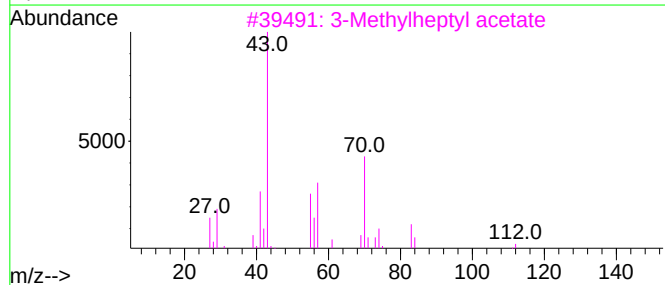
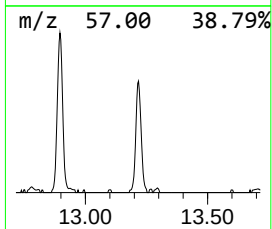
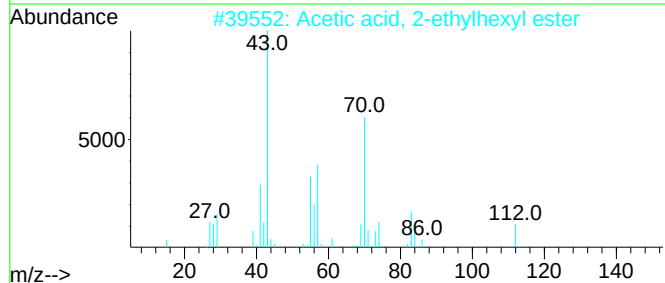
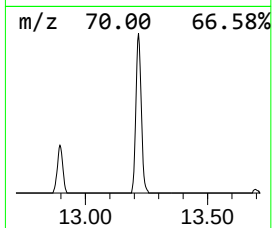
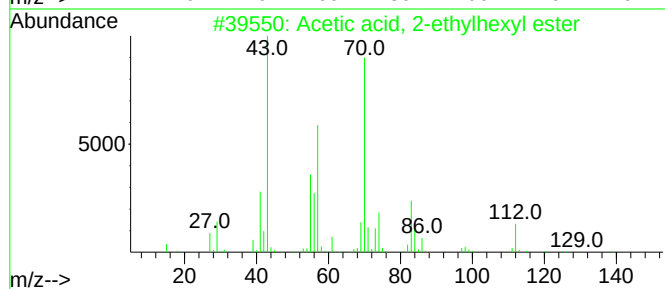
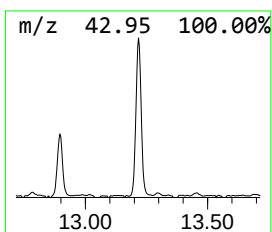
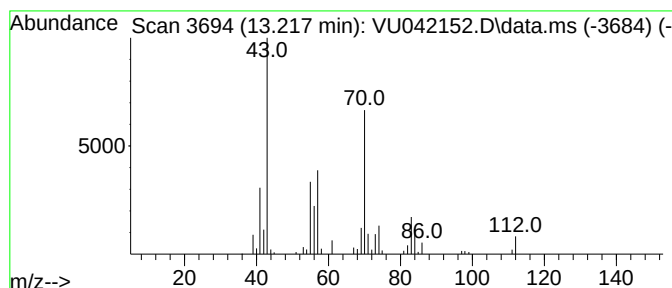
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Acetic acid, 2-ethylhexyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.217	1.19 ug/L	76450	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	91
2			Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	91
3			3-Methylheptyl acetate	172	C10H20O2	072218-58-7	90
4			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	64
5			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	59



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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
Hexanal	8.793	0.9	ug/L	57045	2	9.426	318403	5.0
Octanal	11.697	0.6	ug/L	35402	3	11.819	322313	5.0
1-Hexanol, 2-et...	12.069	1.3	ug/L	81976	3	11.819	322313	5.0
Nonanal	12.896	1.4	ug/L	87792	3	11.819	322313	5.0
Acetic acid, 2-...	13.217	1.2	ug/L	76450	3	11.819	322313	5.0