

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012121\
 Data File : VU042144.D
 Acq On : 21 Jan 2021 12:35
 Operator : SY/MD
 Sample : M1170-13
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFT94

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: VU042144.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	89	rBV	50980	51630	10.24%	1.305%
2	1.916	171	179	193	rVB	38076	47572	9.44%	1.203%
3	2.568	370	382	400	rBV	88603	143582	28.48%	3.630%
4	4.655	1015	1031	1081	rBV	38381	197982	39.28%	5.006%
5	5.073	1146	1161	1178	rBV	77084	169753	33.68%	4.292%
6	5.732	1345	1366	1392	rBV2	155190	407699	80.88%	10.308%
7	6.256	1515	1529	1552	rBV	149132	282598	56.06%	7.145%
8	6.700	1653	1667	1691	rVV2	95951	188053	37.31%	4.755%
9	7.575	1927	1939	1961	rBV	57213	101738	20.18%	2.572%
10	7.906	2029	2042	2059	rBV	189180	324871	64.45%	8.214%
11	8.185	2119	2129	2146	rBV	38419	65286	12.95%	1.651%
12	8.645	2258	2272	2303	rBV	264744	504069	100.00%	12.745%
13	8.796	2308	2319	2340	rVB2	19626	34777	6.90%	0.879%
14	9.427	2502	2515	2531	rBV	199933	332864	66.04%	8.416%
15	10.353	2791	2803	2817	rBV2	13038	20565	4.08%	0.520%
16	10.764	2920	2931	2945	rVB	77117	123300	24.46%	3.118%
17	11.697	3210	3221	3233	rBV2	35120	54374	10.79%	1.375%
18	11.819	3247	3259	3277	rVB	205053	321380	63.76%	8.126%
19	12.070	3326	3337	3358	rBV2	26119	51465	10.21%	1.301%
20	12.201	3367	3378	3394	rVB	180544	291241	57.78%	7.364%
21	12.896	3582	3594	3606	rBV	112778	167494	33.23%	4.235%
22	13.992	3922	3935	3947	rBV4	6709	9616	1.91%	0.243%
23	14.459	4069	4080	4093	rBV2	9886	14188	2.81%	0.359%
24	15.410	4364	4376	4385	rBV	30602	43577	8.65%	1.102%
25	16.304	4648	4654	4661	rVB6	4149	5379	1.07%	0.136%

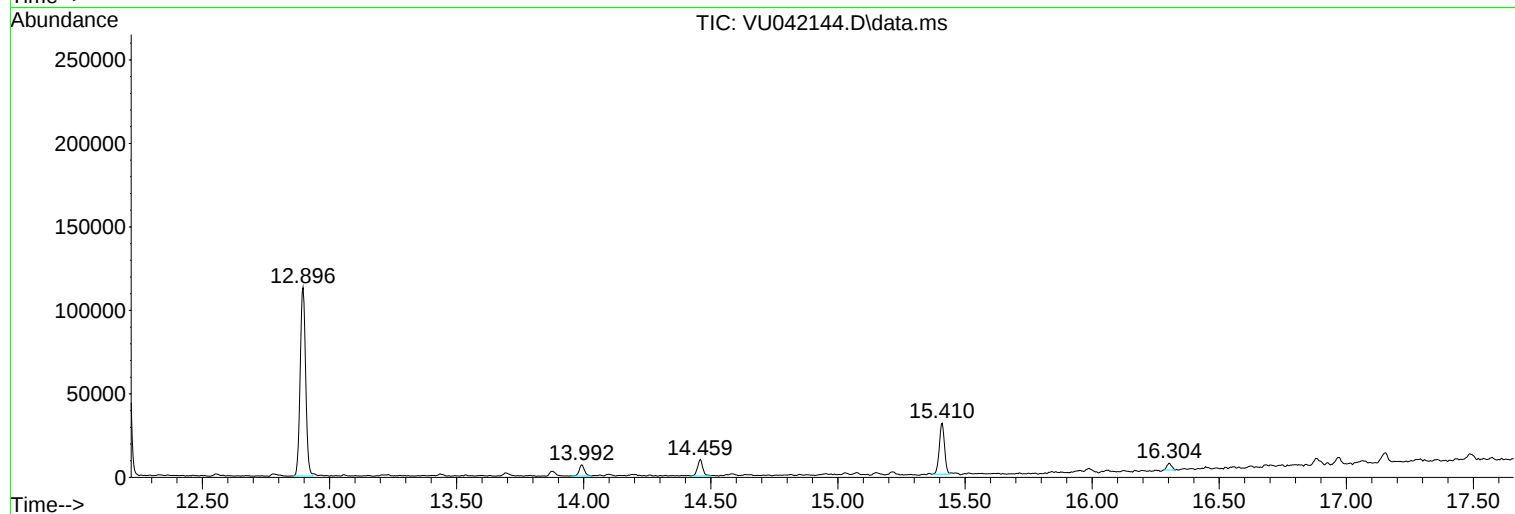
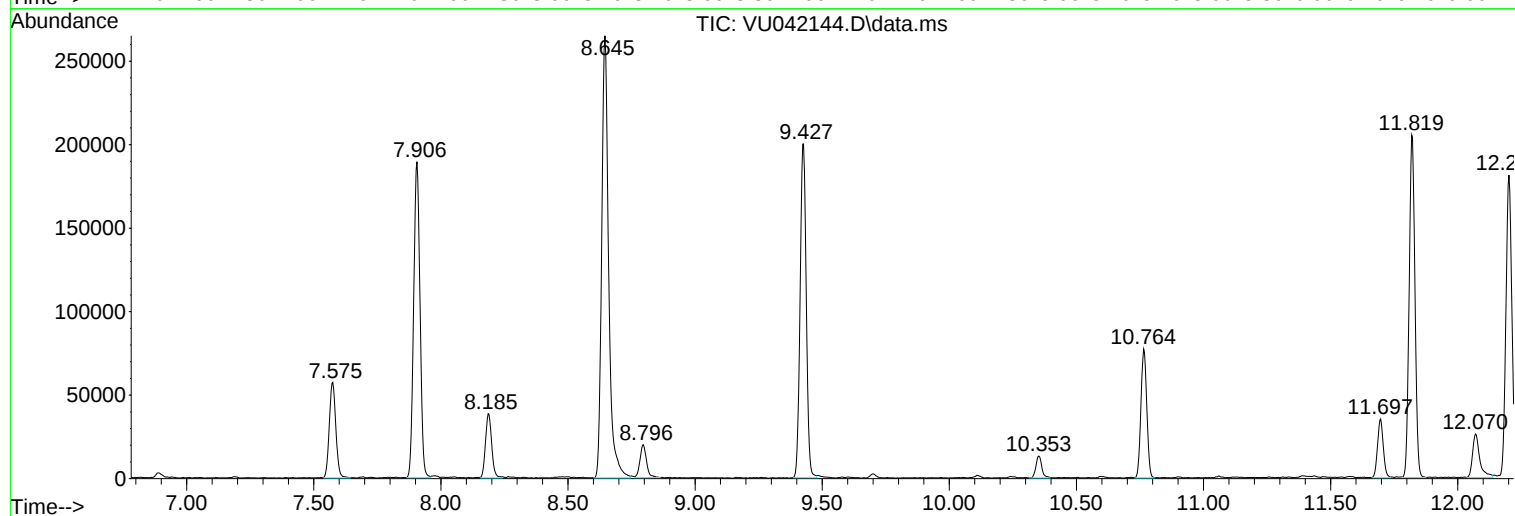
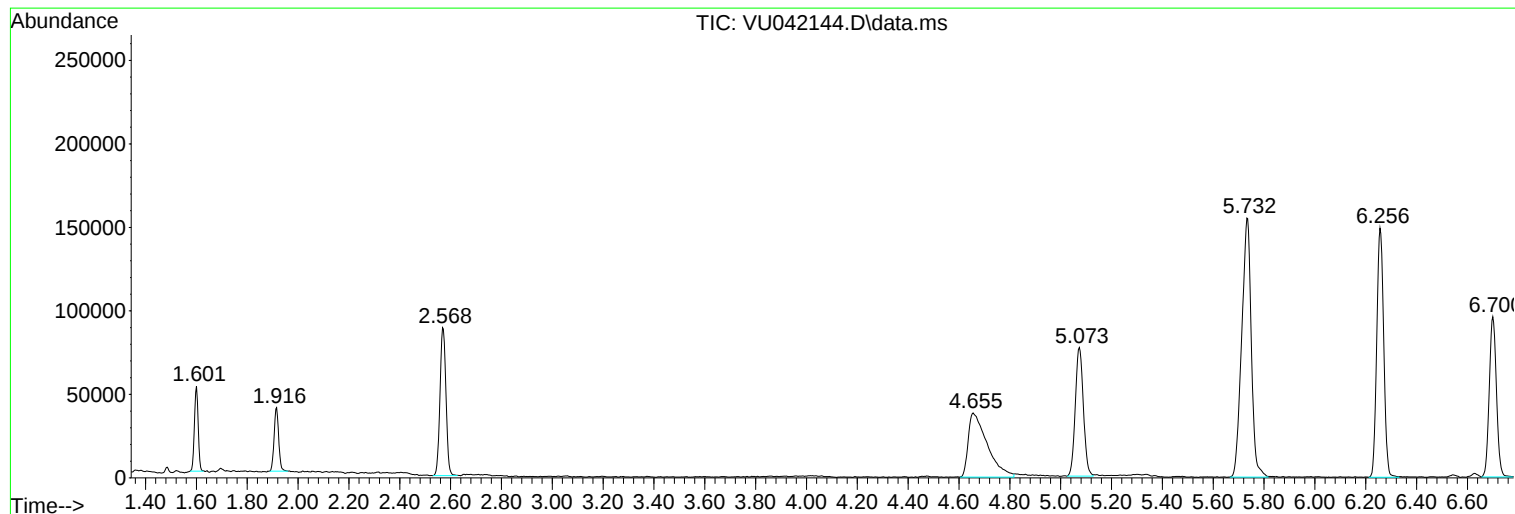
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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



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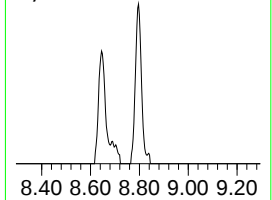
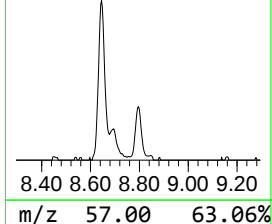
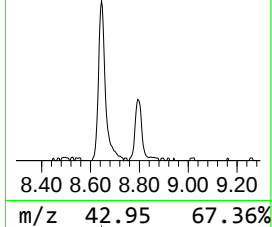
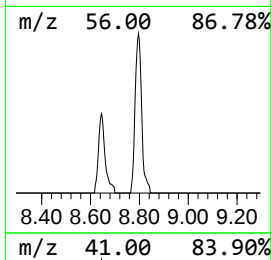
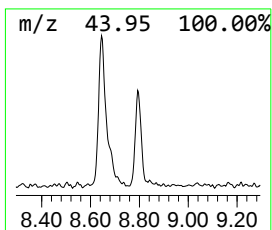
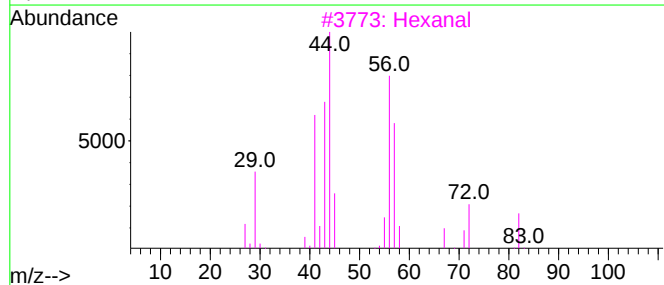
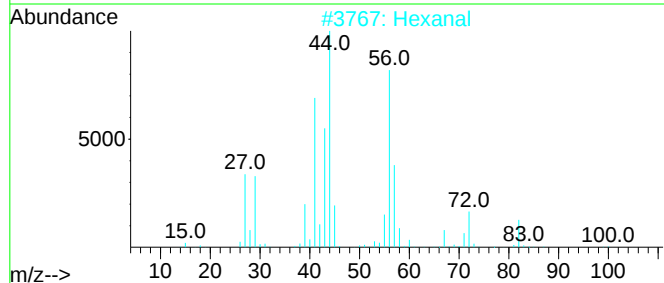
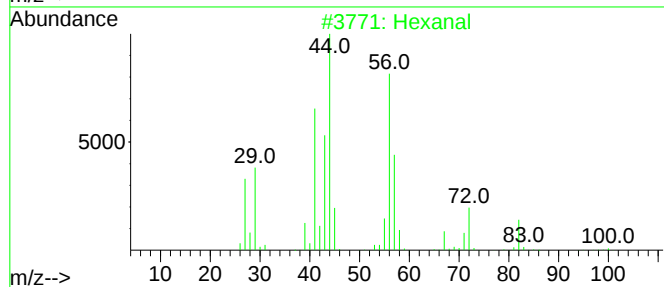
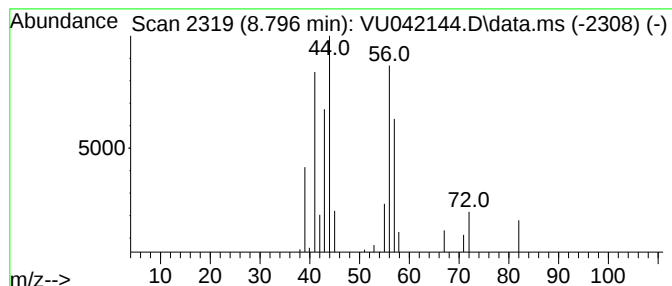
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.796	0.52 ug/L	34777	Chlorobenzene-d5	9.427

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



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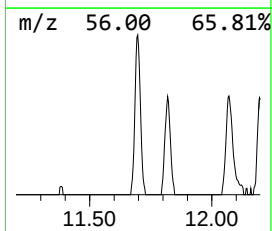
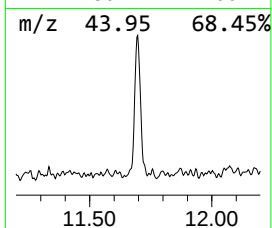
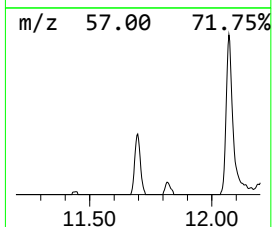
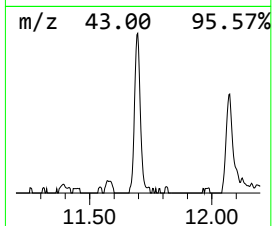
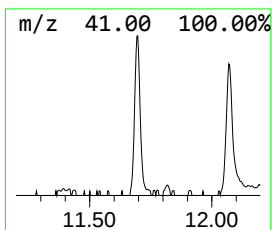
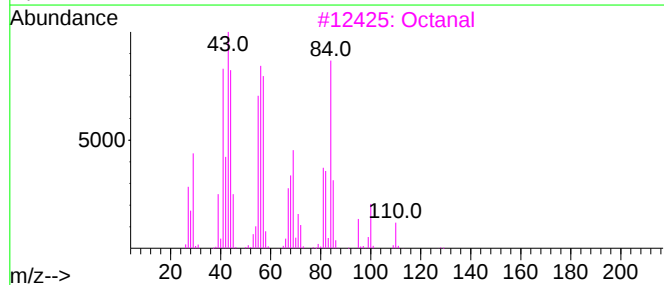
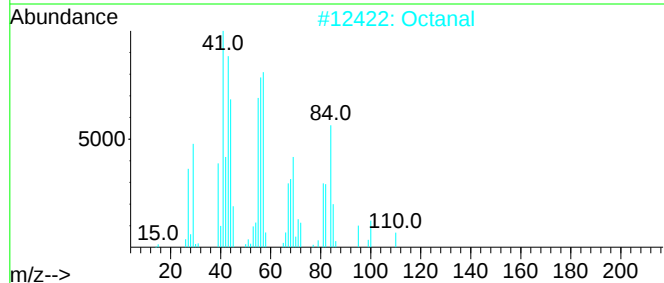
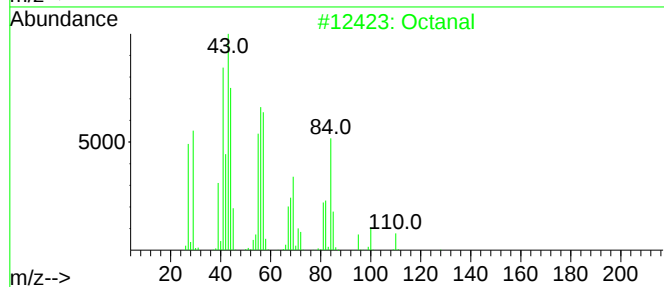
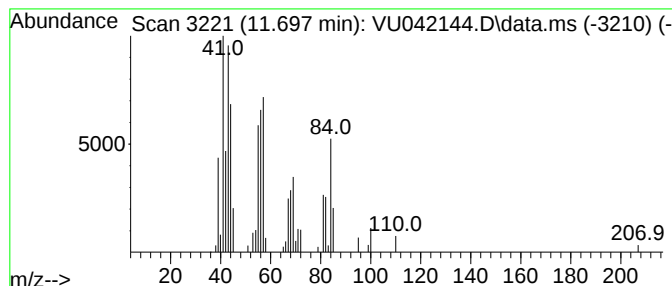
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.697	0.85 ug/L	54374	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	91
3	Octanal			128	C8H16O	000124-13-0	91
4	Octanal			128	C8H16O	000124-13-0	87
5	Octanal			128	C8H16O	000124-13-0	72



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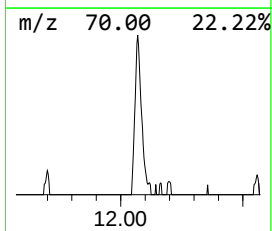
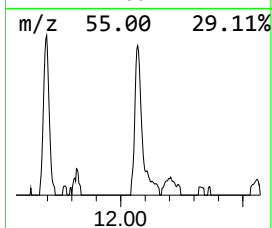
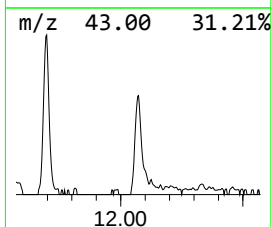
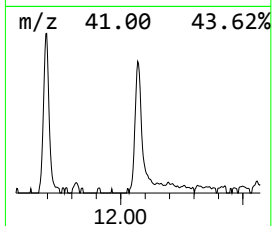
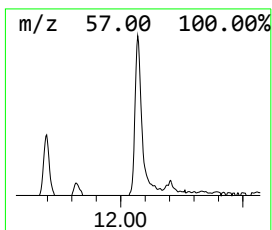
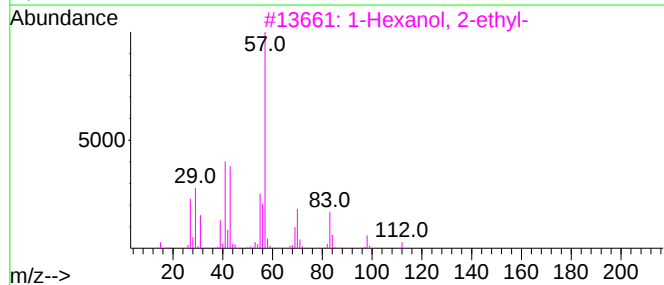
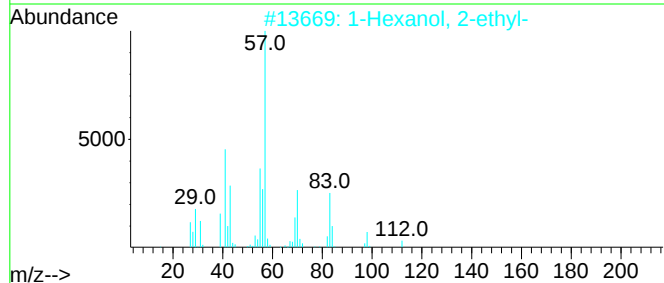
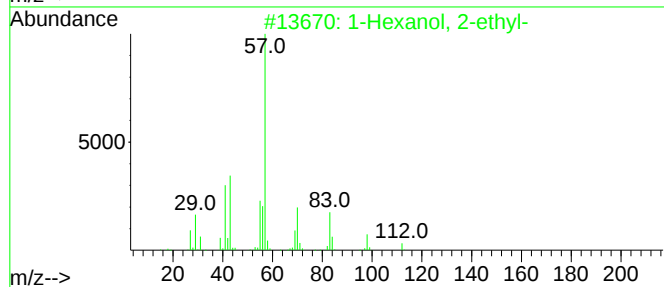
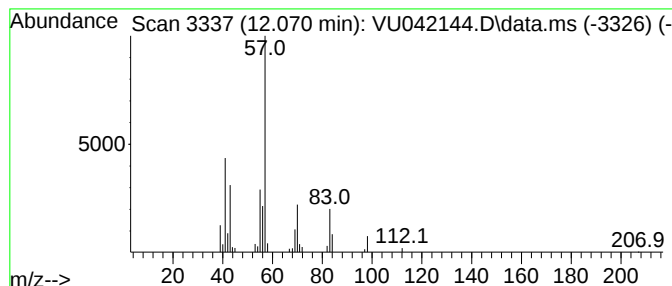
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.070	0.80 ug/L	51465	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	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	64
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53



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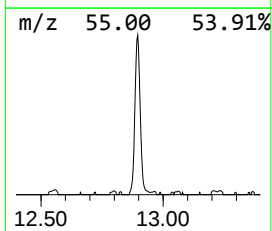
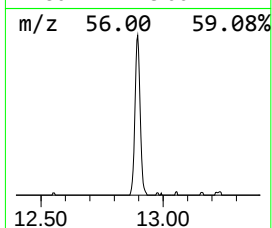
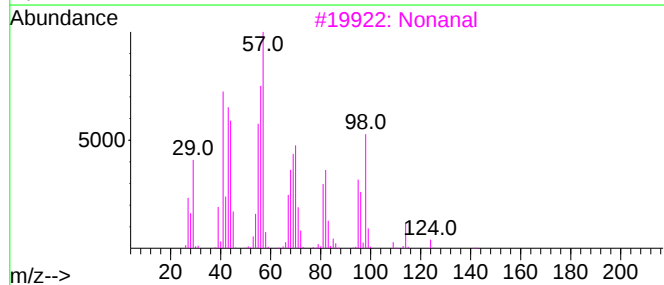
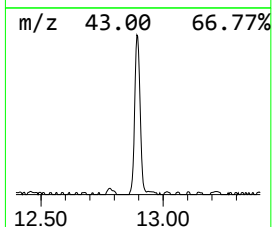
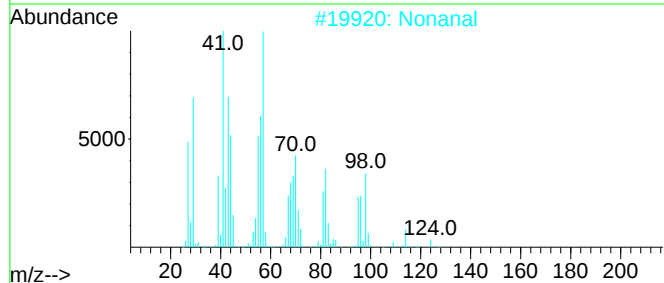
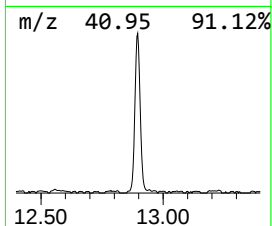
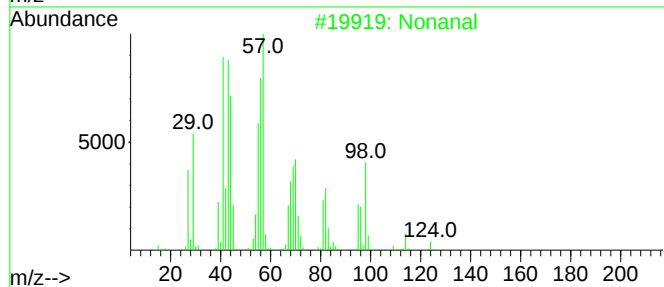
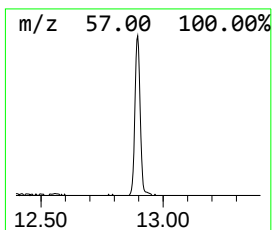
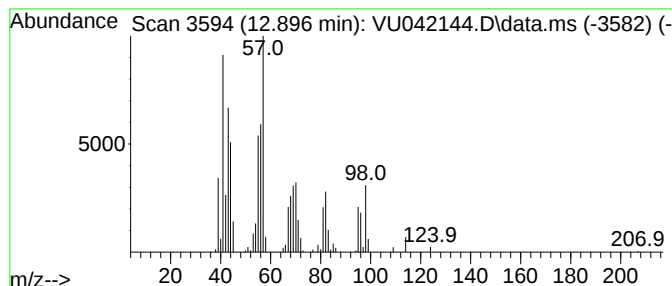
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.896	2.61 ug/L	167494	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	91
3			Nonanal	142	C9H18O	000124-19-6	91
4			Nonanal	142	C9H18O	000124-19-6	91
5			2-Heptene	98	C7H14	000592-77-8	30



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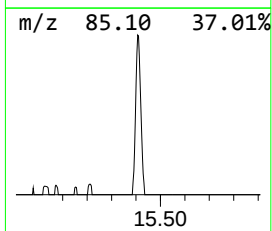
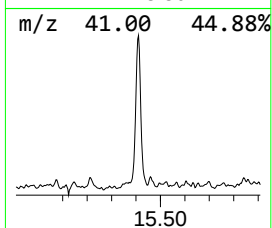
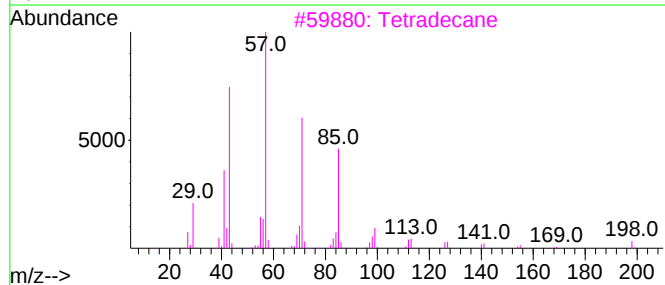
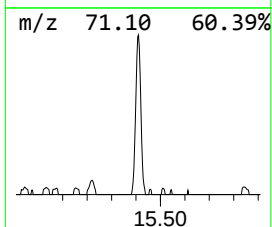
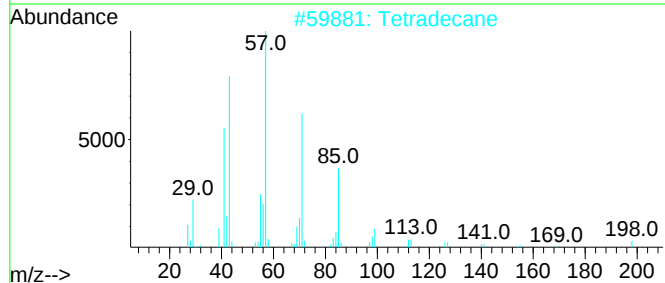
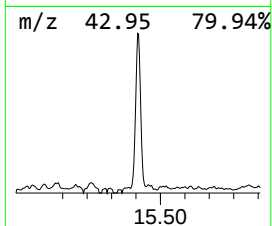
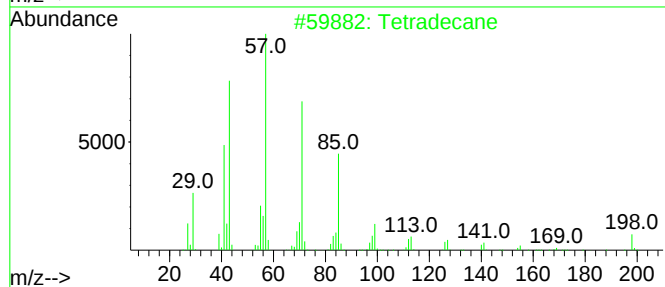
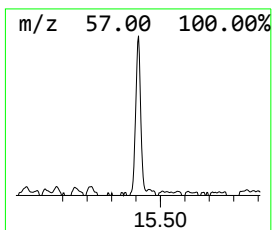
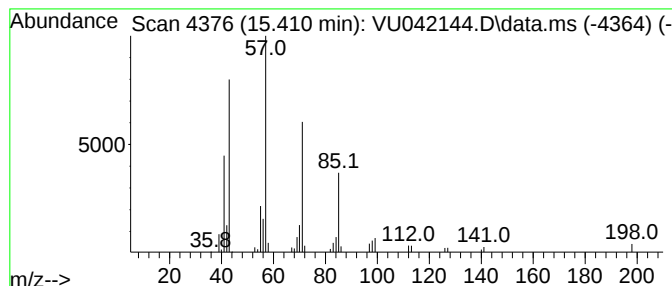
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	0.68 ug/L	43577	1,4-Dichlorobenzene-d4	11.819

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecane	198	C14H30	000629-59-4	97
2		Tetradecane	198	C14H30	000629-59-4	96
3		Tetradecane	198	C14H30	000629-59-4	96
4		Tetradecane	198	C14H30	000629-59-4	95
5		Tridecane	184	C13H28	000629-50-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.796	0.5	ug/L	34777	2	9.427	332864	5.0
Octanal	11.697	0.8	ug/L	54374	3	11.819	321380	5.0
1-Hexanol, 2-et...	12.070	0.8	ug/L	51465	3	11.819	321380	5.0
Nonanal	12.896	2.6	ug/L	167494	3	11.819	321380	5.0
(DEL) Alkane: S...	15.410	0.7	ug/L	43577	3	11.819	321380	5.0