

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070323\
 Data File : VU054752.D
 Acq On : 03 Jul 2023 16:29
 Operator : MD/SY
 Sample : 03505-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A46R9

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\SFAMUTR060723WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU054752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	88	95	111	rBV	80792	97544	9.70%	1.036%
2	1.904	184	191	205	rVB	72274	100369	9.98%	1.066%
3	2.560	383	395	407	rBV	141416	231504	23.03%	2.458%
4	2.631	407	417	445	rVB	79054	152038	15.12%	1.614%
5	3.039	530	544	561	rBV	57342	114181	11.36%	1.212%
6	3.181	569	588	609	rVB	153247	346910	34.51%	3.684%
7	4.624	1022	1037	1060	rBV2	220698	610291	60.70%	6.480%
8	4.821	1090	1098	1118	rVB3	7738	19604	1.95%	0.208%
9	5.058	1156	1172	1192	rVB2	149980	339872	33.81%	3.609%
10	5.721	1358	1378	1405	rBV2	288436	787846	78.36%	8.366%
11	6.245	1528	1541	1569	rBV	307765	611098	60.78%	6.489%
12	6.541	1623	1633	1643	rBV8	7643	14894	1.48%	0.158%
13	6.689	1662	1679	1695	rBV	190236	381847	37.98%	4.055%
14	6.885	1731	1740	1755	rBV6	8670	17751	1.77%	0.188%
15	7.563	1938	1951	1970	rBV	90747	170365	16.95%	1.809%
16	7.795	2013	2023	2032	rBV3	5517	10418	1.04%	0.111%
17	7.894	2041	2054	2066	rBV	319416	563842	56.08%	5.987%
18	7.968	2066	2077	2103	rVB	358366	642135	63.87%	6.818%
19	8.177	2130	2142	2160	rBV2	59002	107135	10.66%	1.138%
20	8.554	2247	2259	2271	rVB2	22209	39269	3.91%	0.417%
21	8.631	2271	2283	2320	rBV	525063	1005387	100.00%	10.676%
22	8.785	2320	2331	2354	rVB	98853	178281	17.73%	1.893%
23	9.415	2514	2527	2546	rBV	441599	746281	74.23%	7.924%
24	9.499	2546	2553	2562	rVV6	5924	10310	1.03%	0.109%
25	9.570	2565	2575	2591	rVB3	14890	26789	2.66%	0.284%
26	9.692	2602	2613	2626	rBV3	35056	60491	6.02%	0.642%
27	10.103	2727	2741	2756	rBV6	24083	53313	5.30%	0.566%
28	10.235	2771	2782	2795	rBV3	7013	12195	1.21%	0.129%
29	10.344	2800	2816	2827	rVV4	20159	35439	3.52%	0.376%
30	10.566	2871	2885	2904	rBV4	13001	25850	2.57%	0.274%
31	10.753	2931	2943	2958	rBV	165402	269226	26.78%	2.859%
32	10.891	2977	2986	3000	rBV2	8766	18374	1.83%	0.195%
33	11.470	3156	3166	3174	rBV6	12890	21894	2.18%	0.232%
34	11.685	3223	3233	3243	rBV4	26183	42382	4.22%	0.450%
35	11.811	3259	3272	3286	rBV	439116	705375	70.16%	7.490%
36	11.904	3292	3301	3316	rVB	6835	14776	1.47%	0.157%

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Title : TRACE VOA SFAM1.0

37	12.061	3340	3350	3370	rBV3	28830	77392	7.70%	0.822%
38	12.190	3377	3390	3406	rBV	336635	544725	54.18%	5.784%
39	12.528	3484	3495	3504	rBV3	24875	47170	4.69%	0.501%
40	12.885	3597	3606	3624	rVB2	67861	104137	10.36%	1.106%
41	13.685	3842	3855	3865	rBV2	4813	11985	1.19%	0.127%
42	14.775	4187	4194	4204	rVB3	8450	13147	1.31%	0.140%
43	14.978	4245	4257	4271	rBV7	14496	23476	2.34%	0.249%
44	15.692	4471	4479	4488	rVB8	6166	10363	1.03%	0.110%

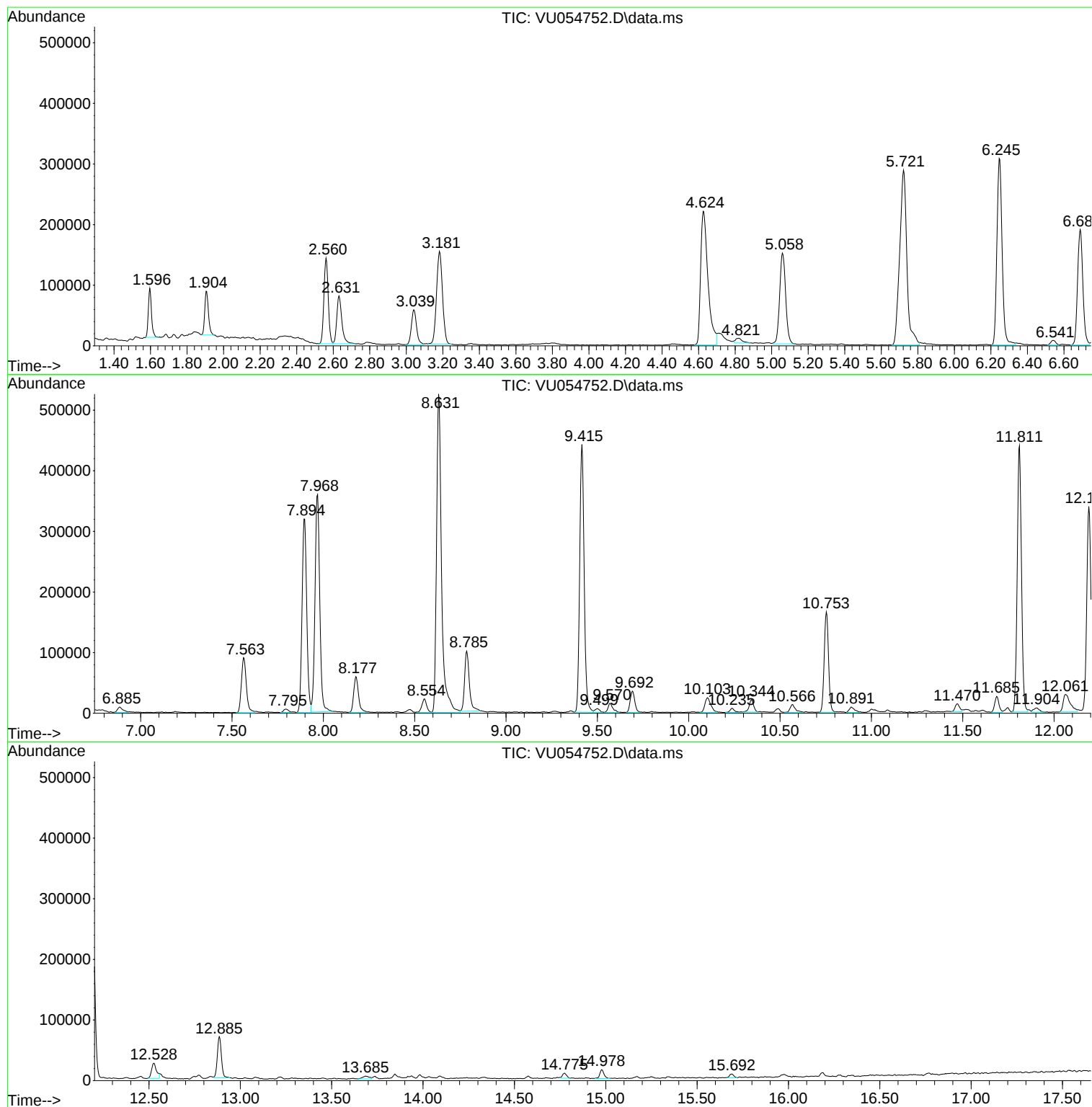
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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A46R9

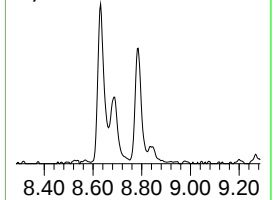
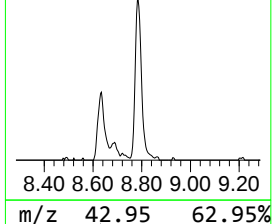
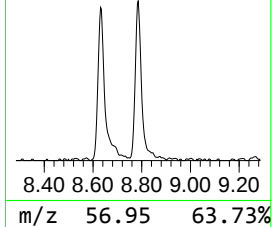
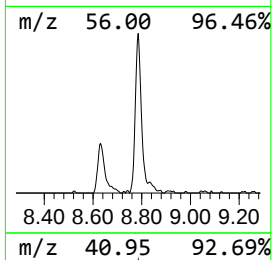
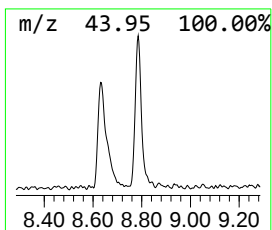
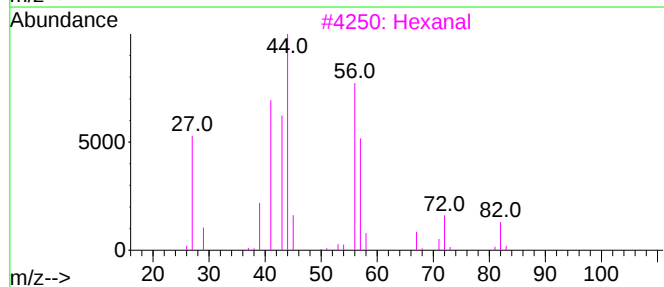
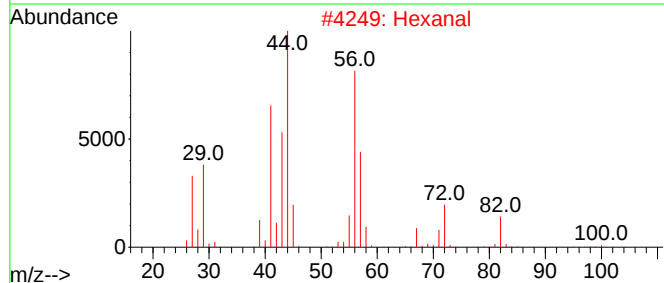
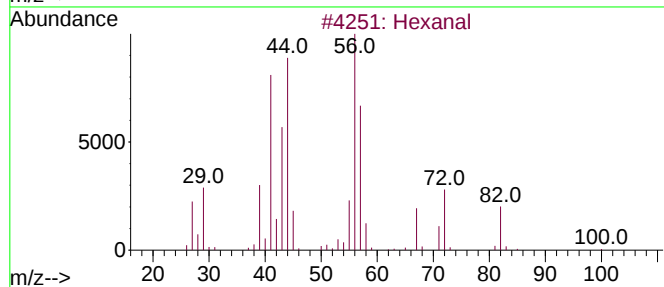
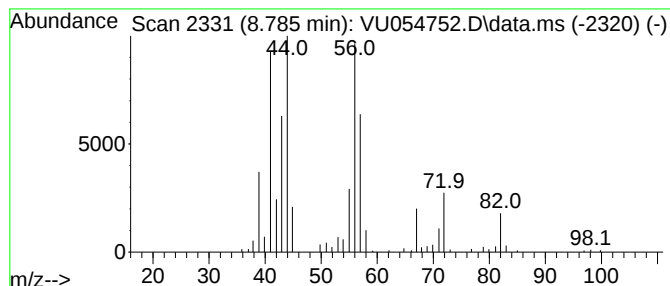
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	1.19 ug/L	178281	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	93
2	Hexanal			100	C6H12O	000066-25-1	90
3	Hexanal			100	C6H12O	000066-25-1	86
4	Hexanal			100	C6H12O	000066-25-1	80
5	Hexanal			100	C6H12O	000066-25-1	78



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A46R9

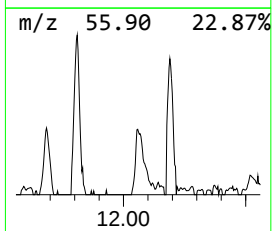
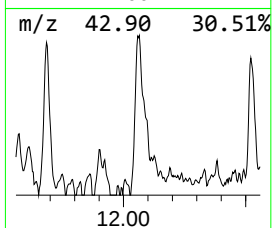
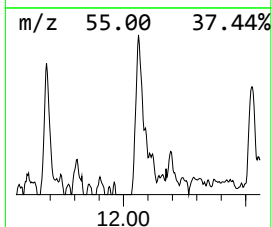
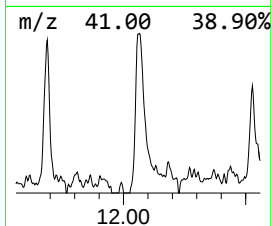
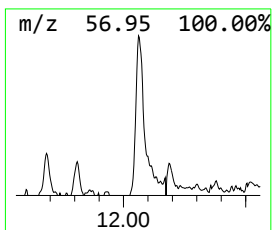
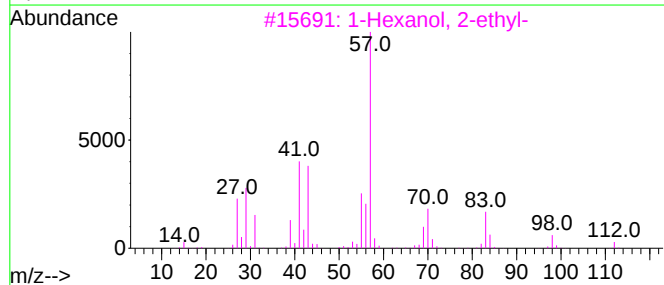
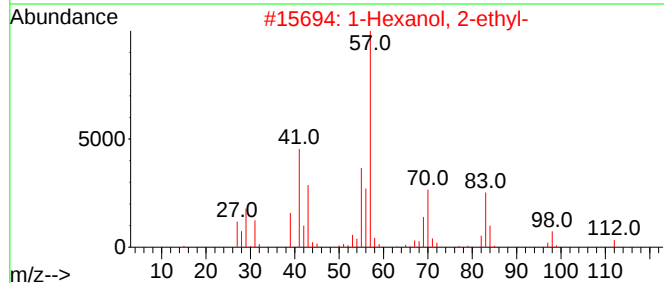
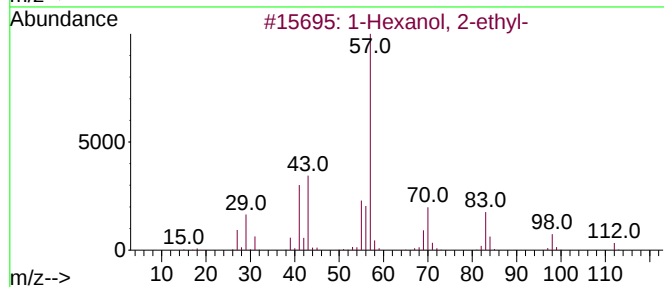
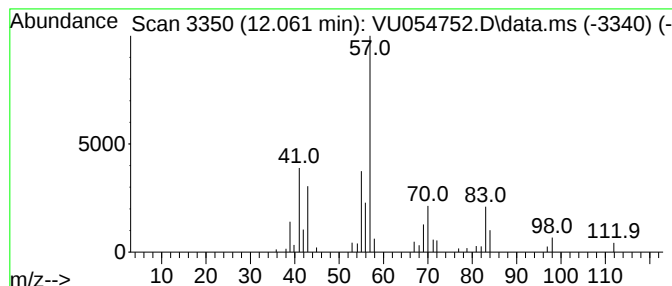
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	0.55 ug/L	77392	1,4-Dichlorobenzene-d4	11.811

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	83
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Isobutoxy-2-ethylhexane			186	C12H26O	1000139-90-3	53



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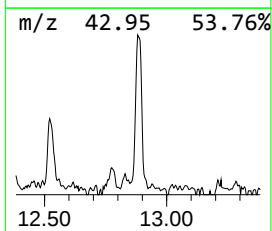
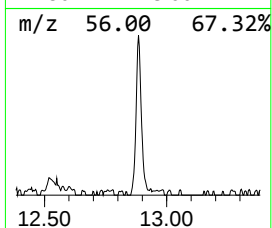
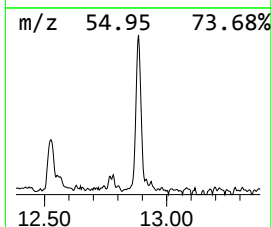
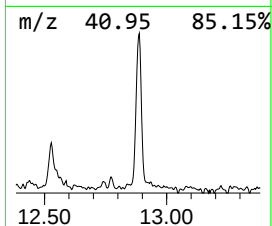
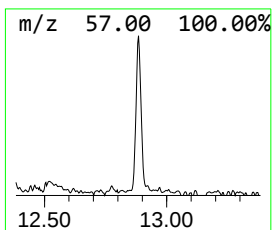
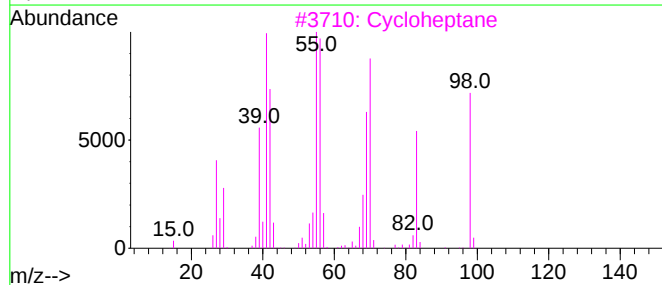
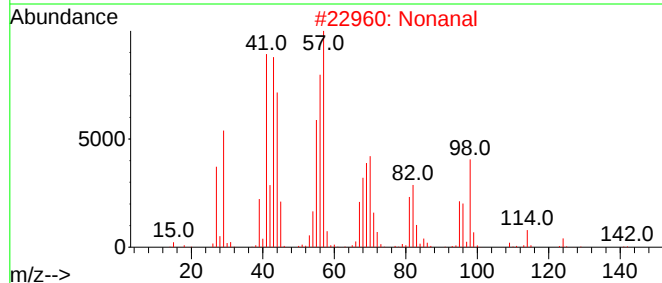
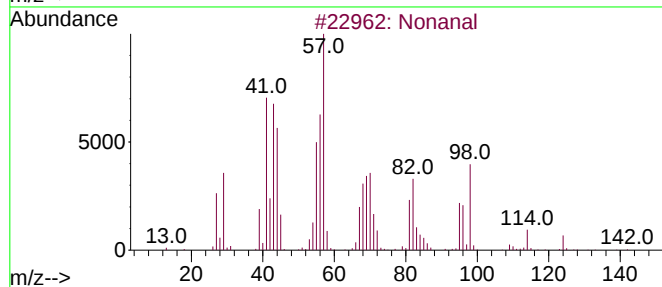
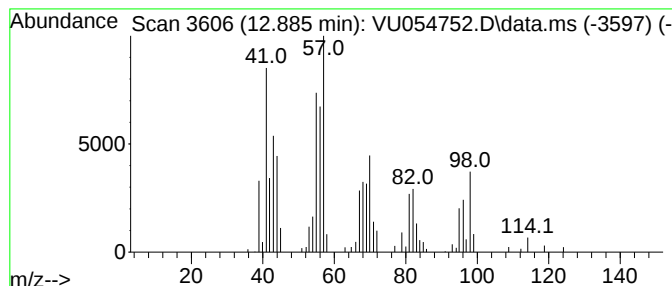
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	0.74 ug/L	104137	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	83
2			Nonanal	142	C9H18O	000124-19-6	78
3			Cycloheptane	98	C7H14	000291-64-5	38
4			Cycloheptane	98	C7H14	000291-64-5	35
5			Cycloheptane	98	C7H14	000291-64-5	35



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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.785	1.2	ug/L	178281	2	9.415	746281	5.0
1-Hexanol, 2-et...	12.061	0.6	ug/L	77392	3	11.811	705375	5.0
Nonanal	12.884	0.7	ug/L	104137	3	11.811	705375	5.0