

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070323\
 Data File : VU054753.D
 Acq On : 03 Jul 2023 16:54
 Operator : MD/SY
 Sample : 03505-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A46T2

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: VU054753.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	87	95	109	rBV	86314	108640	10.57%	1.132%
2	1.904	184	191	207	rVB	75392	109195	10.63%	1.138%
3	2.560	384	395	407	rBV	147722	234631	22.83%	2.445%
4	2.631	407	417	436	rVB	109364	196374	19.11%	2.047%
5	2.792	454	467	477	rBV4	5514	11595	1.13%	0.121%
6	3.039	530	544	558	rBV	33035	64904	6.32%	0.676%
7	3.181	572	588	608	rVB	96886	224171	21.81%	2.336%
8	4.624	1023	1037	1059	rBV2	205062	546702	53.20%	5.698%
9	5.058	1157	1172	1196	rVB	157277	359823	35.01%	3.750%
10	5.721	1358	1378	1408	rBV2	294215	816896	79.49%	8.513%
11	6.248	1528	1542	1559	rBV	337805	649784	63.23%	6.772%
12	6.689	1664	1679	1696	rBV2	198655	395679	38.50%	4.124%
13	6.885	1728	1740	1752	rBV5	7585	16259	1.58%	0.169%
14	7.563	1940	1951	1965	rBV	96541	170263	16.57%	1.774%
15	7.897	2041	2055	2066	rBV	335821	589997	57.41%	6.149%
16	7.968	2066	2077	2106	rVB	402161	719563	70.02%	7.499%
17	8.177	2130	2142	2160	rBV2	61888	111783	10.88%	1.165%
18	8.470	2219	2233	2244	rBV3	9264	16259	1.58%	0.169%
19	8.550	2246	2258	2272	rBV5	16281	31159	3.03%	0.325%
20	8.631	2272	2283	2311	rBV	550859	1027684	100.00%	10.710%
21	8.785	2321	2331	2345	rBV	88684	148205	14.42%	1.545%
22	9.415	2515	2527	2547	rBV	475940	804008	78.23%	8.379%
23	9.569	2567	2575	2591	rVB2	13766	25209	2.45%	0.263%
24	9.692	2599	2613	2627	rBV2	34641	60441	5.88%	0.630%
25	10.100	2727	2740	2758	rVB5	21042	48191	4.69%	0.502%
26	10.238	2773	2783	2794	rBV2	5650	10538	1.03%	0.110%
27	10.344	2805	2816	2830	rVB4	18760	30661	2.98%	0.320%
28	10.566	2873	2885	2896	rBV3	15965	27017	2.63%	0.282%
29	10.753	2930	2943	2959	rBV	167069	277506	27.00%	2.892%
30	10.891	2976	2986	3003	rBV	16965	30075	2.93%	0.313%
31	11.470	3156	3166	3175	rBV3	12826	22662	2.21%	0.236%
32	11.685	3224	3233	3245	rBV4	23457	39032	3.80%	0.407%
33	11.811	3259	3272	3289	rBV	476568	760273	73.98%	7.923%
34	12.065	3339	3351	3377	rBV3	31067	89711	8.73%	0.935%
35	12.190	3378	3390	3406	rVB	351672	569972	55.46%	5.940%
36	12.524	3484	3494	3516	rBV4	31096	65827	6.41%	0.686%

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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

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Title : TRACE VOA SFAM1.0

37	12.884	3597	3606	3625	rVB2	63664	100290	9.76%	1.045%
38	13.855	3896	3908	3917	rBV2	6071	12705	1.24%	0.132%
39	14.775	4187	4194	4203	rVB4	10309	15668	1.52%	0.163%
40	14.981	4248	4258	4269	rVB4	18004	30024	2.92%	0.313%
41	15.688	4469	4478	4487	rBV7	8107	12809	1.25%	0.133%
42	15.978	4560	4568	4581	rVB10	7647	13205	1.28%	0.138%

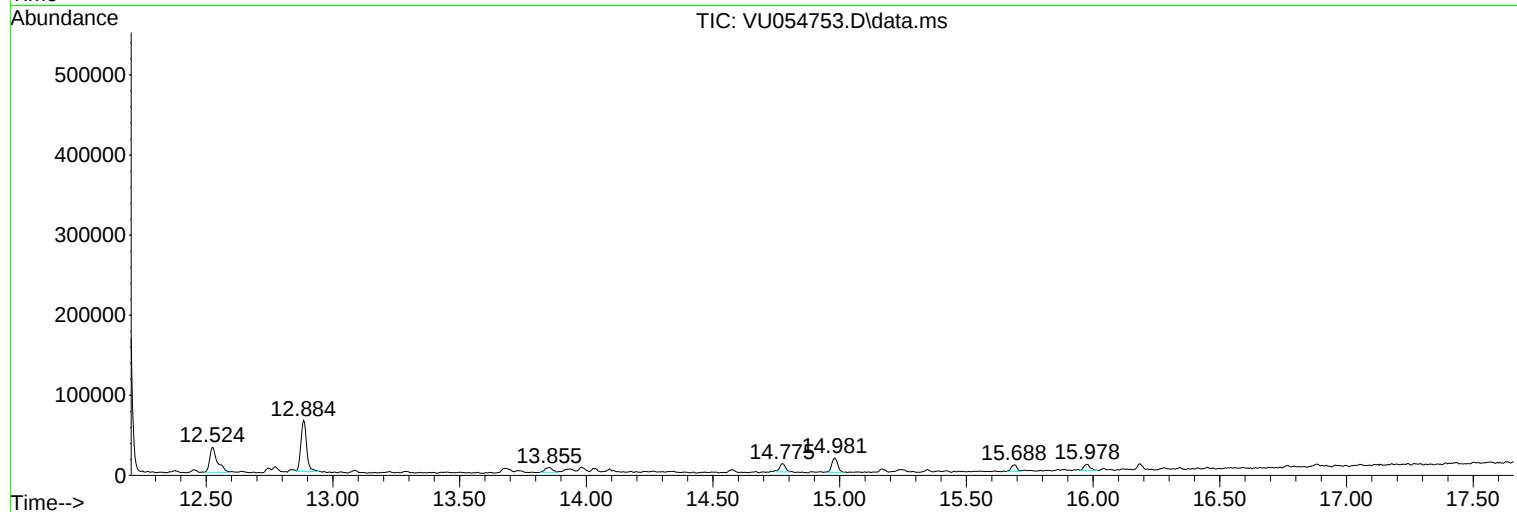
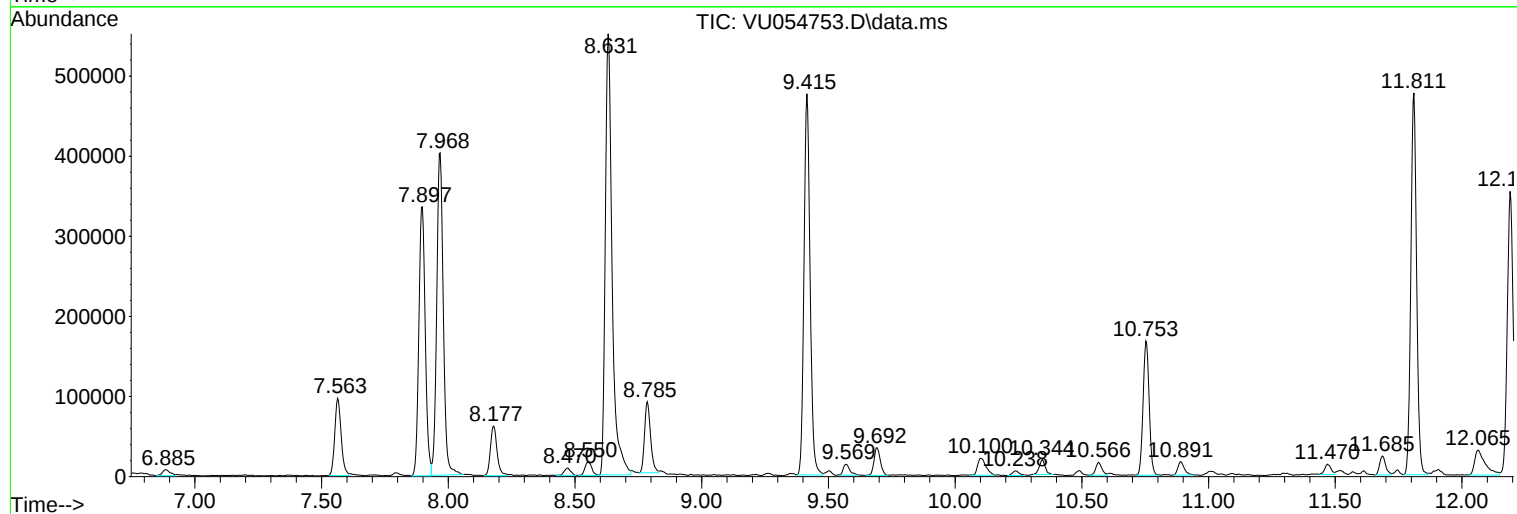
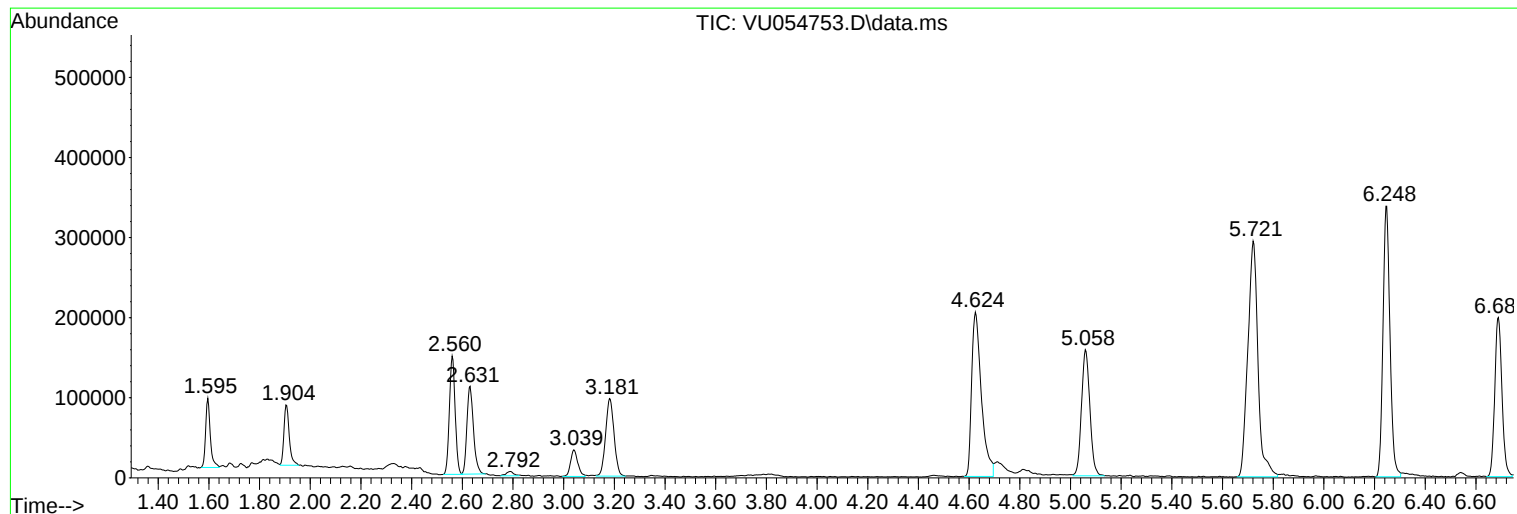
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
MSVOA_U
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A46T2

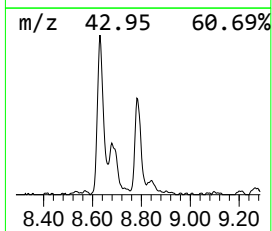
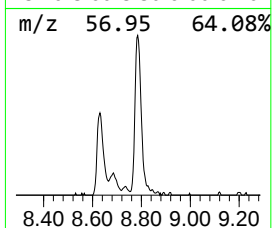
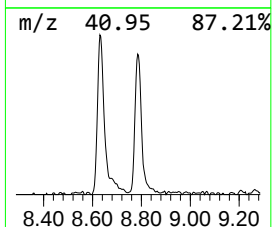
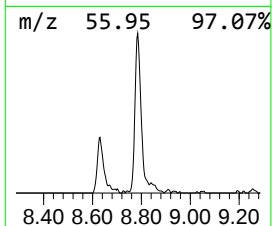
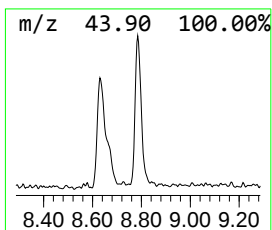
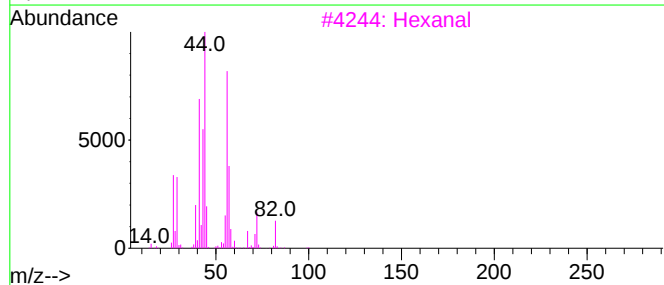
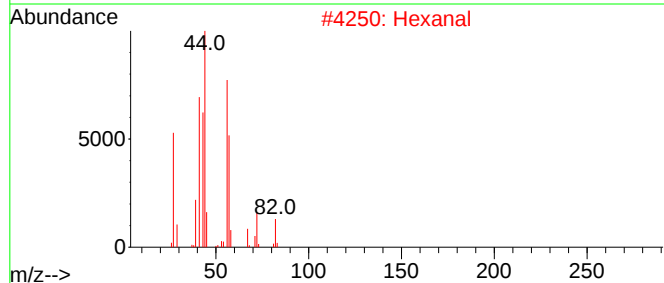
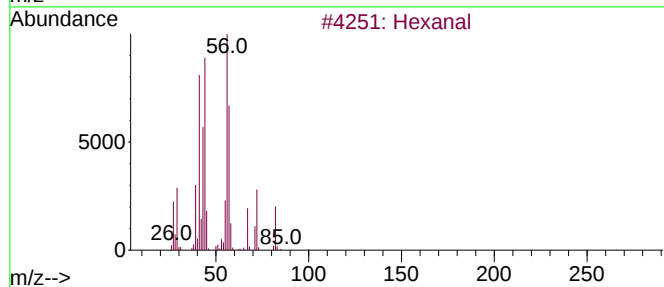
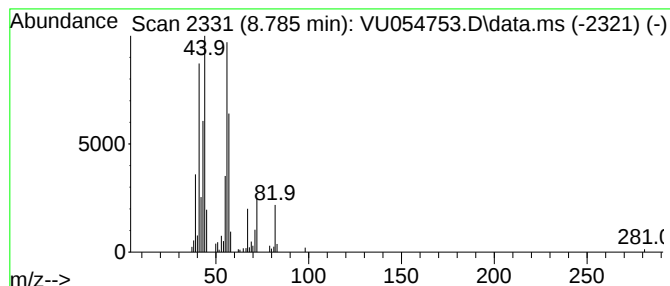
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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	0.92 ug/L	148205	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	72
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	72
5	Hexanal			100	C6H12O	000066-25-1	64



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A46T2

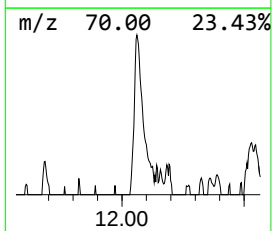
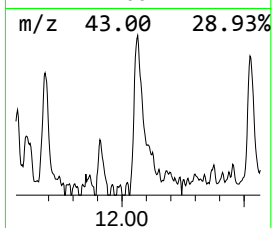
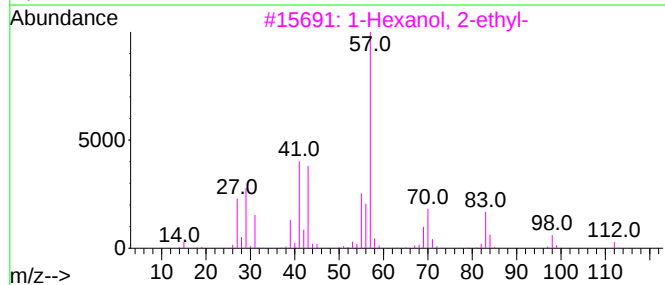
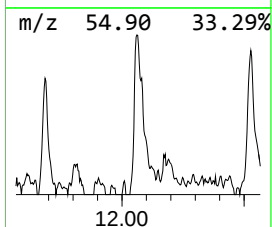
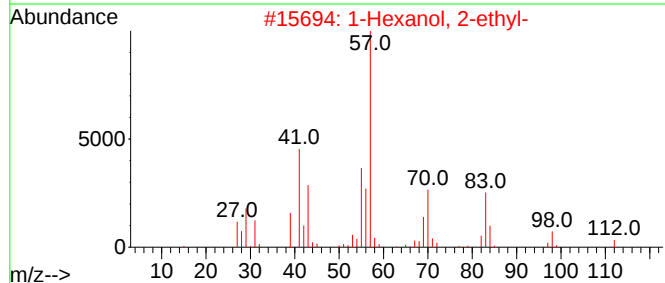
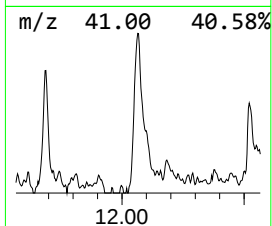
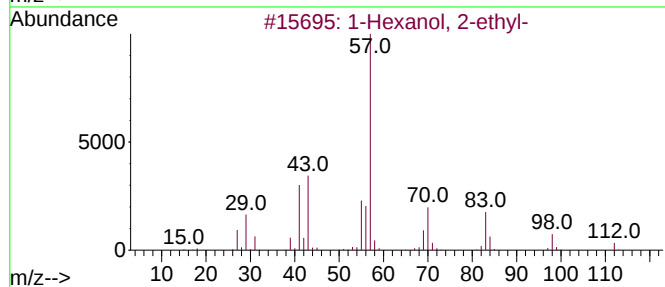
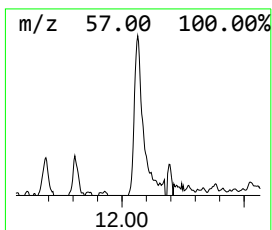
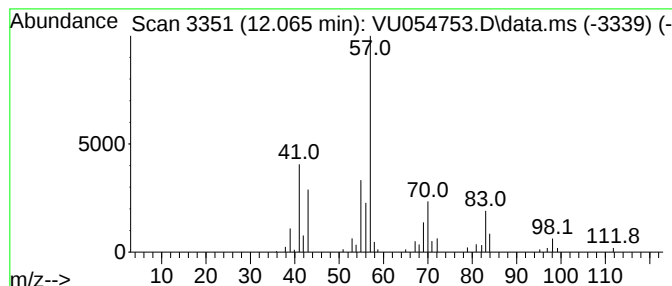
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
12.065	0.59 ug/L	89711	1,4-Dichlorobenzene-d4	11.810

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	72
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72



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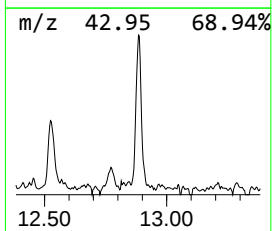
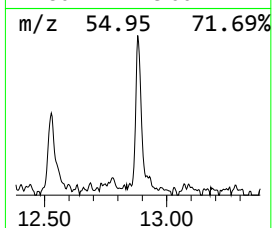
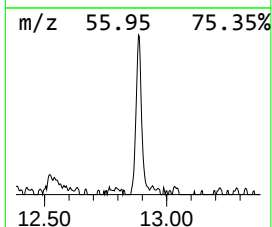
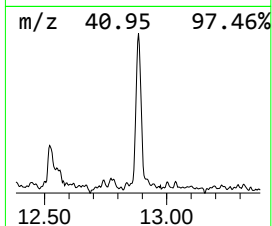
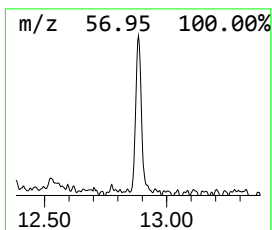
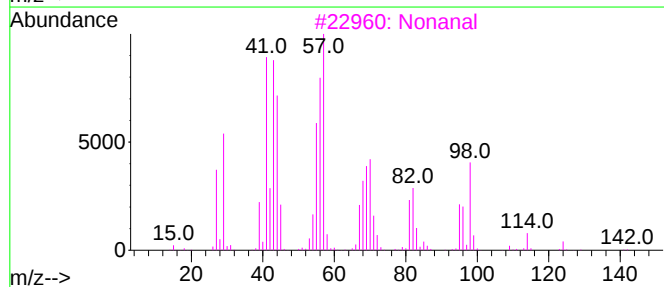
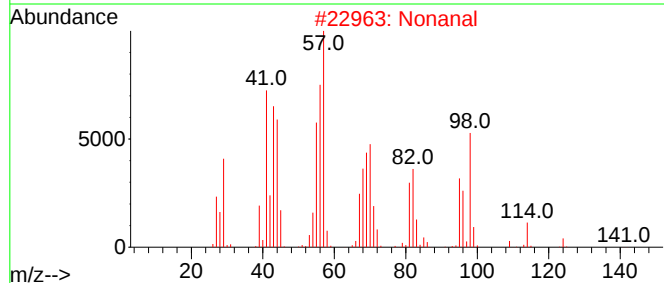
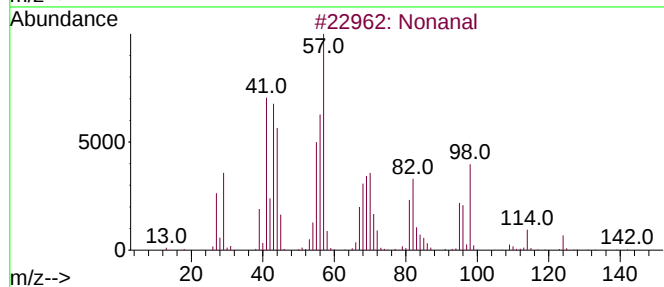
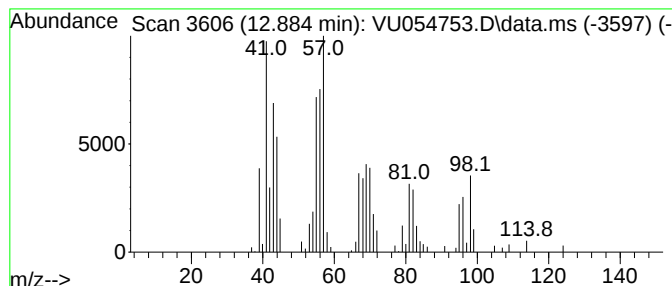
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Quant Title : TRACE VOA SFAM1.0

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	0.66 ug/L	100290	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	90
2			Nonanal	142	C9H18O	000124-19-6	78
3			Nonanal	142	C9H18O	000124-19-6	72
4			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	38
5			(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	38



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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	0.9	ug/L	148205	2	9.415	804008	5.0
1-Hexanol, 2-et...	12.065	0.6	ug/L	89711	3	11.810	760273	5.0
Nonanal	12.884	0.7	ug/L	100290	3	11.810	760273	5.0