

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070323\
 Data File : VU054755.D
 Acq On : 03 Jul 2023 17:43
 Operator : MD/SY
 Sample : 03505-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A46X9

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: VU054755.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.518	65	71	81	rBV2	10455	18283	1.87%	0.207%
2	1.596	88	95	109	rVB	78399	94849	9.69%	1.071%
3	1.907	184	192	211	rVB	74195	109650	11.20%	1.238%
4	2.560	383	395	406	rBV	134510	217630	22.22%	2.458%
5	2.628	406	416	441	rVB	91823	174575	17.83%	1.972%
6	3.042	533	545	565	rBV2	28759	57066	5.83%	0.645%
7	3.181	574	588	606	rVB	60114	140036	14.30%	1.582%
8	4.624	1022	1037	1059	rBV3	180655	475698	48.58%	5.373%
9	5.058	1154	1172	1192	rBV	149895	332217	33.92%	3.752%
10	5.721	1358	1378	1405	rBV2	275507	750846	76.67%	8.481%
11	6.245	1526	1541	1562	rBV	309302	607203	62.00%	6.858%
12	6.689	1664	1679	1701	rBV	188636	371018	37.89%	4.191%
13	6.885	1729	1740	1750	rBV4	11273	23367	2.39%	0.264%
14	7.563	1938	1951	1970	rBV	90100	163015	16.65%	1.841%
15	7.791	2011	2022	2035	rBV5	6192	11975	1.22%	0.135%
16	7.894	2038	2054	2066	rBV	315418	553377	56.51%	6.250%
17	7.968	2066	2077	2102	rVB	205542	368976	37.68%	4.168%
18	8.177	2127	2142	2156	rBV	58499	99310	10.14%	1.122%
19	8.470	2222	2233	2244	rBV2	7723	13876	1.42%	0.157%
20	8.550	2249	2258	2271	rVB3	12420	22519	2.30%	0.254%
21	8.631	2271	2283	2319	rBV	511055	979286	100.00%	11.061%
22	8.785	2320	2331	2343	rBV2	150961	255650	26.11%	2.888%
23	9.415	2514	2527	2548	rBV	445823	741138	75.68%	8.371%
24	9.570	2564	2575	2591	rVB	24335	39193	4.00%	0.443%
25	9.692	2603	2613	2626	rBV	39781	67623	6.91%	0.764%
26	10.110	2730	2743	2764	rVB5	35951	87352	8.92%	0.987%
27	10.235	2774	2782	2793	rBV	24994	37184	3.80%	0.420%
28	10.341	2800	2815	2827	rBV5	24688	44083	4.50%	0.498%
29	10.566	2875	2885	2899	rBV4	15037	28999	2.96%	0.328%
30	10.753	2931	2943	2959	rBV	159311	260559	26.61%	2.943%
31	10.891	2977	2986	3008	rVB	15574	30244	3.09%	0.342%
32	11.470	3158	3166	3174	rBV5	13314	21089	2.15%	0.238%
33	11.685	3223	3233	3244	rVV4	29142	49870	5.09%	0.563%
34	11.746	3244	3252	3258	rVV7	7156	10755	1.10%	0.121%
35	11.807	3258	3271	3291	rVV	440713	727120	74.25%	8.213%
36	11.901	3292	3300	3317	rVB	8028	17858	1.82%	0.202%

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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	12.065	3337	3351	3370	rBV3	25752	72016	7.35%	0.813%
38	12.190	3378	3390	3410	rVB	322647	529610	54.08%	5.982%
39	12.524	3484	3494	3521	rBV2	33970	72013	7.35%	0.813%
40	12.885	3597	3606	3617	rVV2	79716	119806	12.23%	1.353%
41	14.775	4186	4194	4204	rVB4	8048	13668	1.40%	0.154%
42	14.981	4249	4258	4272	rBV4	17554	26496	2.71%	0.299%
43	15.688	4469	4478	4486	rBV4	10199	16528	1.69%	0.187%

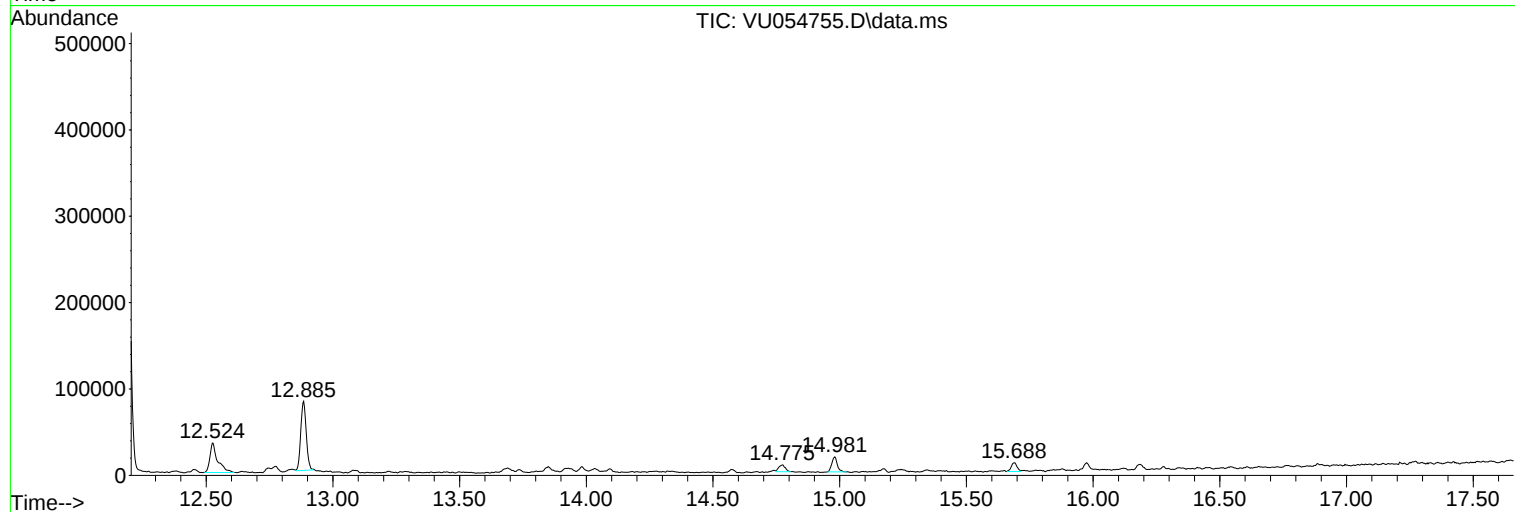
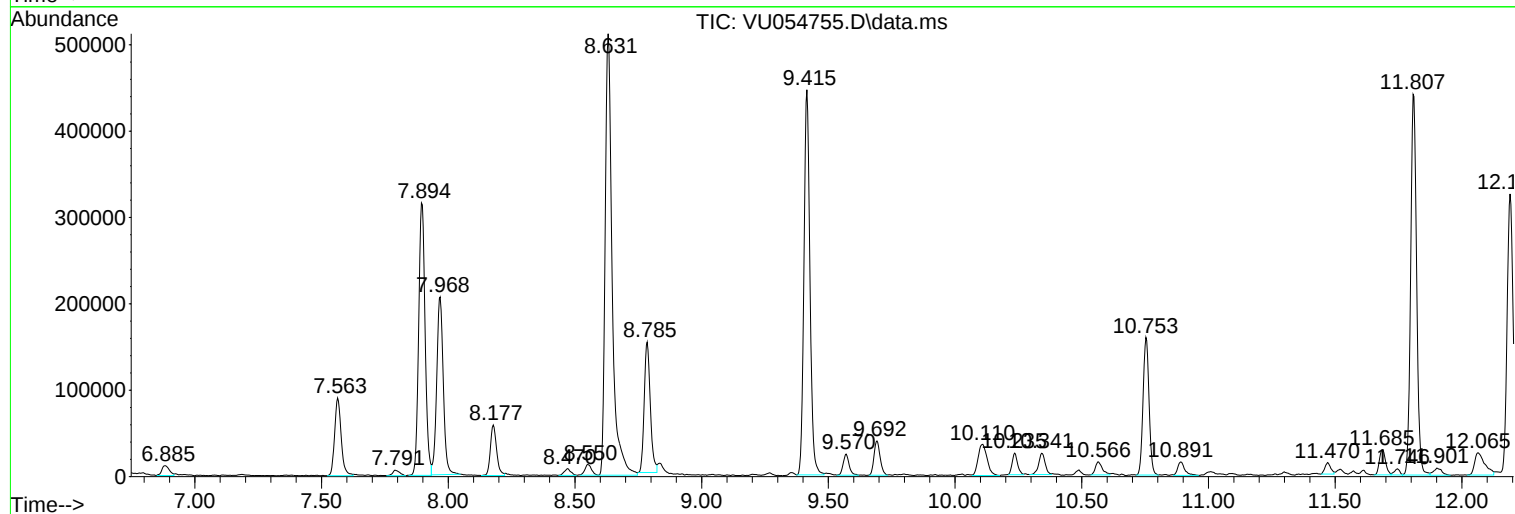
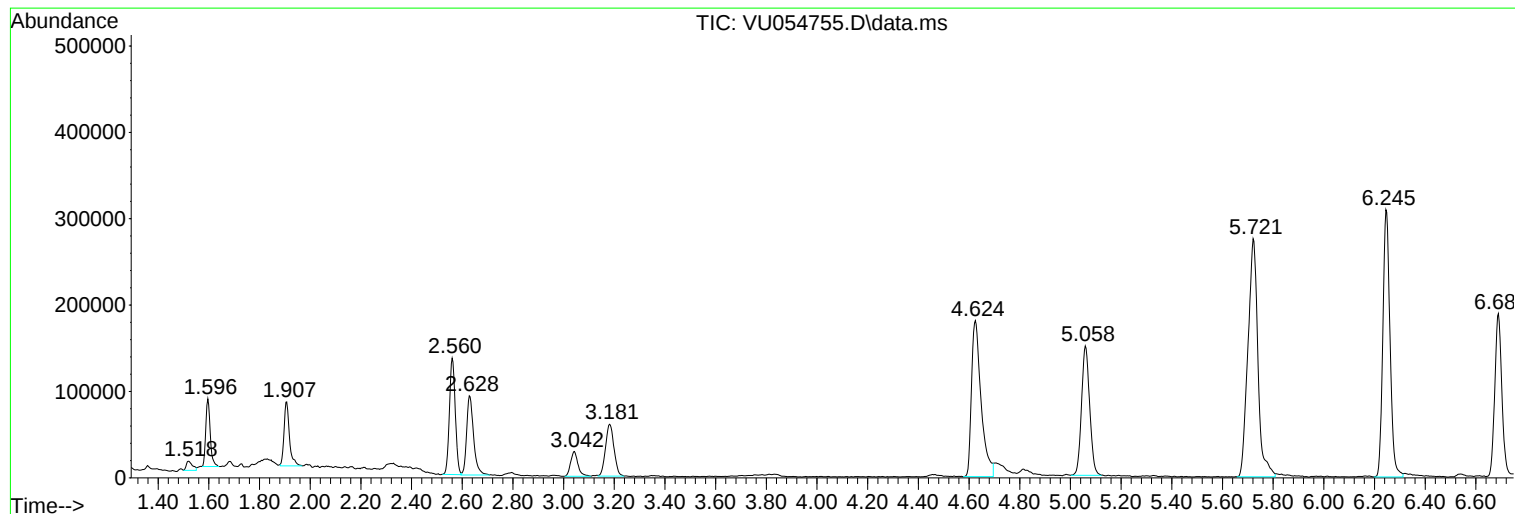
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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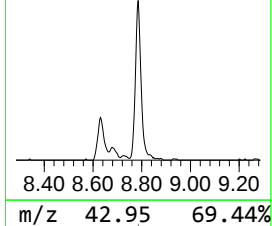
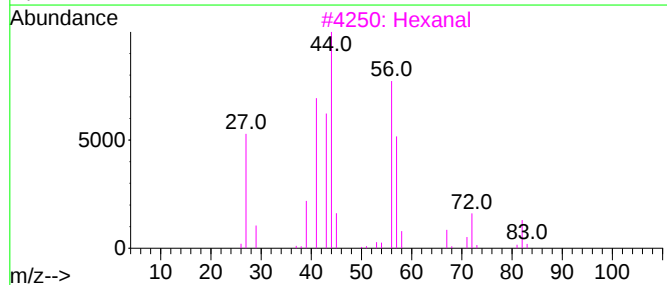
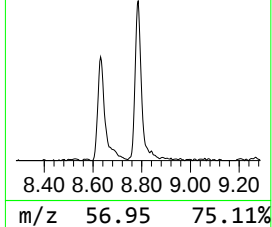
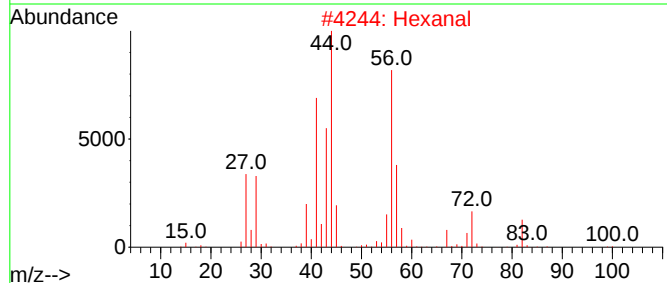
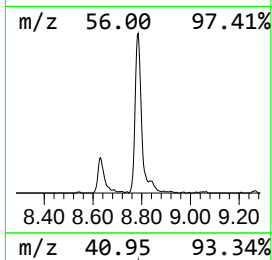
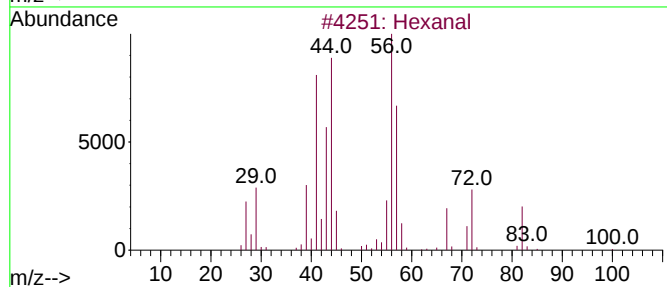
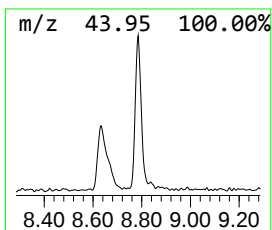
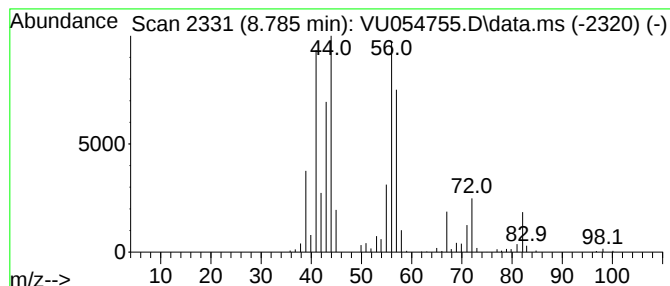
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Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	1.72 ug/L	255650	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	95
2	Hexanal			100	C6H12O	000066-25-1	90
3	Hexanal			100	C6H12O	000066-25-1	86
4	Hexanal			100	C6H12O	000066-25-1	78
5	Hexanal			100	C6H12O	000066-25-1	78



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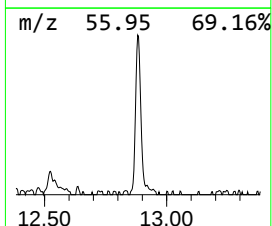
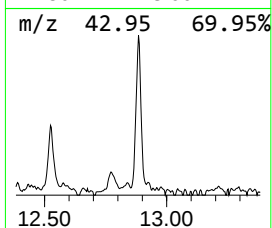
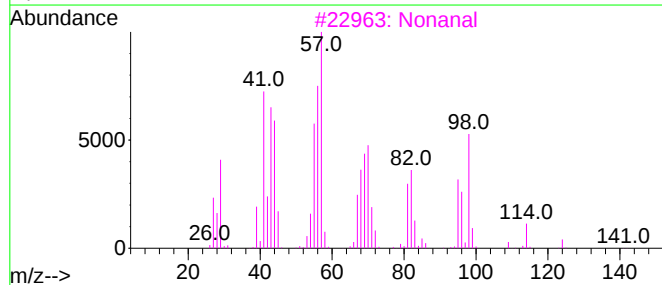
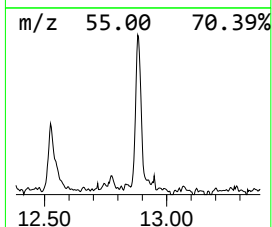
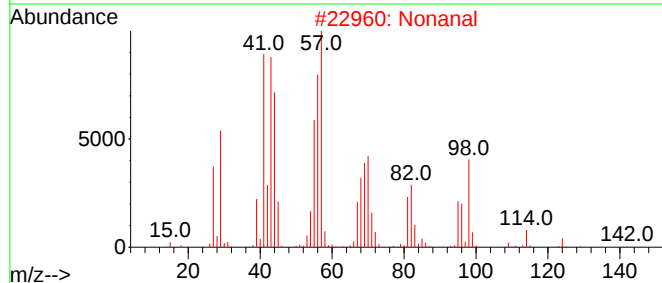
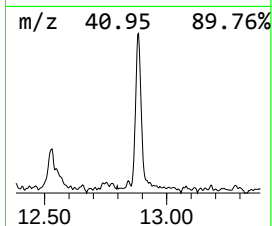
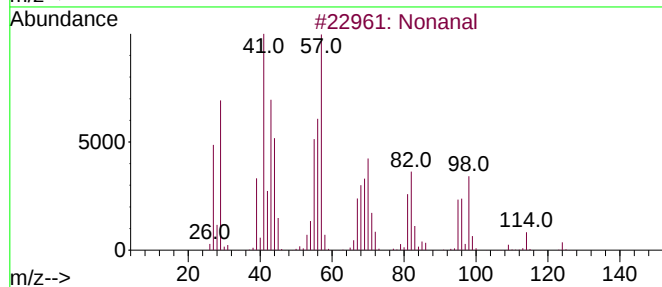
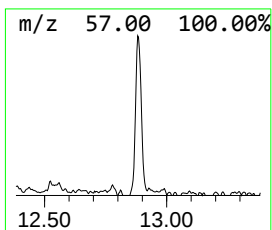
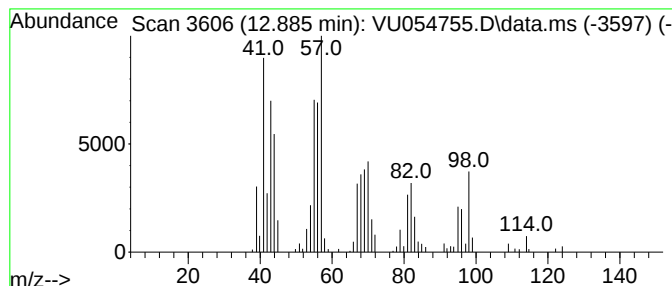
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.884	0.82 ug/L	119806	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal			142	C9H18O	000124-19-6	90
2	Nonanal			142	C9H18O	000124-19-6	90
3	Nonanal			142	C9H18O	000124-19-6	90
4	Nonanal			142	C9H18O	000124-19-6	80
5	2-Nonen-1-ol, (E)-			142	C9H18O	031502-14-4	35



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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.785	1.7	ug/L	255650	2	9.415	741138	5.0
Nonanal	12.884	0.8	ug/L	119806	3	11.807	727120	5.0