

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102723\
 Data File : VU055920.D
 Acq On : 27 Oct 2023 12:36
 Operator : MD/SY
 Sample : 05009-17
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4A52

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\SFAMUTR102423WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU055920.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.522	60	72	81	rBV2	34788	94842	6.73%	0.714%
2	1.599	89	96	113	rVB	178146	207489	14.72%	1.563%
3	1.914	186	194	213	rVB	143476	201797	14.32%	1.520%
4	2.567	385	397	408	rBV	300733	491108	34.84%	3.699%
5	2.634	408	418	456	rVB	109112	275500	19.55%	2.075%
6	3.046	532	546	558	rBV2	8536	17091	1.21%	0.129%
7	3.184	565	589	609	rBV	37769	94762	6.72%	0.714%
8	4.458	973	985	996	rBV3	8584	21729	1.54%	0.164%
9	4.628	1020	1038	1058	rBV2	184576	550481	39.06%	4.146%
10	5.059	1156	1172	1201	rBV	266212	604666	42.90%	4.555%
11	5.724	1357	1379	1410	rBV2	542992	1409450	100.00%	10.617%
12	6.245	1525	1541	1563	rBV	468803	961395	68.21%	7.242%
13	6.686	1664	1678	1702	rBV	322487	645120	45.77%	4.859%
14	6.882	1730	1739	1757	rBV2	25625	52066	3.69%	0.392%
15	7.564	1939	1951	1967	rBV	128491	236917	16.81%	1.785%
16	7.792	2011	2022	2038	rBV2	27421	53740	3.81%	0.405%
17	7.895	2041	2054	2071	rVV	672396	1197155	84.94%	9.018%
18	7.969	2073	2077	2096	rVB3	18210	31828	2.26%	0.240%
19	8.178	2130	2142	2157	rBV2	74050	135270	9.60%	1.019%
20	8.473	2222	2234	2243	rBV4	8985	16885	1.20%	0.127%
21	8.631	2270	2283	2321	rBV2	609846	1307842	92.79%	9.851%
22	8.785	2321	2331	2361	rVV	132563	258487	18.34%	1.947%
23	9.416	2514	2527	2553	rBV	652768	1151263	81.68%	8.672%
24	9.599	2578	2584	2595	rVB2	9207	14219	1.01%	0.107%
25	9.692	2605	2613	2626	rVB2	8834	15849	1.12%	0.119%
26	10.104	2730	2741	2747	rBV8	7614	14276	1.01%	0.108%
27	10.235	2773	2782	2797	rBV2	27825	48354	3.43%	0.364%
28	10.342	2805	2815	2828	rBV3	36076	63022	4.47%	0.475%
29	10.573	2875	2887	2904	rBV3	8744	20099	1.43%	0.151%
30	10.753	2927	2943	2961	rBV	227189	380460	26.99%	2.866%
31	10.891	2976	2986	3002	rBV2	19903	36697	2.60%	0.276%
32	11.470	3158	3166	3181	rVB3	14371	25032	1.78%	0.189%
33	11.686	3222	3233	3245	rBV5	46437	79245	5.62%	0.597%
34	11.808	3259	3271	3291	rVB	677025	1102517	78.22%	8.305%
35	12.065	3337	3351	3369	rBV3	40779	106765	7.57%	0.804%
36	12.190	3378	3390	3410	rVB	612972	1013819	71.93%	7.637%

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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\SFAMUTR102423WMA.M
Title : TRACE VOA SFAM1.0

37	12.528	3486	3495	3501	rBV6	9244	15875	1.13%	0.120%
38	12.885	3596	3606	3626	rVB2	122266	196927	13.97%	1.483%
39	13.216	3700	3709	3725	rBV2	23124	37669	2.67%	0.284%
40	13.840	3894	3903	3914	rBV4	32224	55283	3.92%	0.416%
41	14.329	4045	4055	4067	rVB	19570	32843	2.33%	0.247%

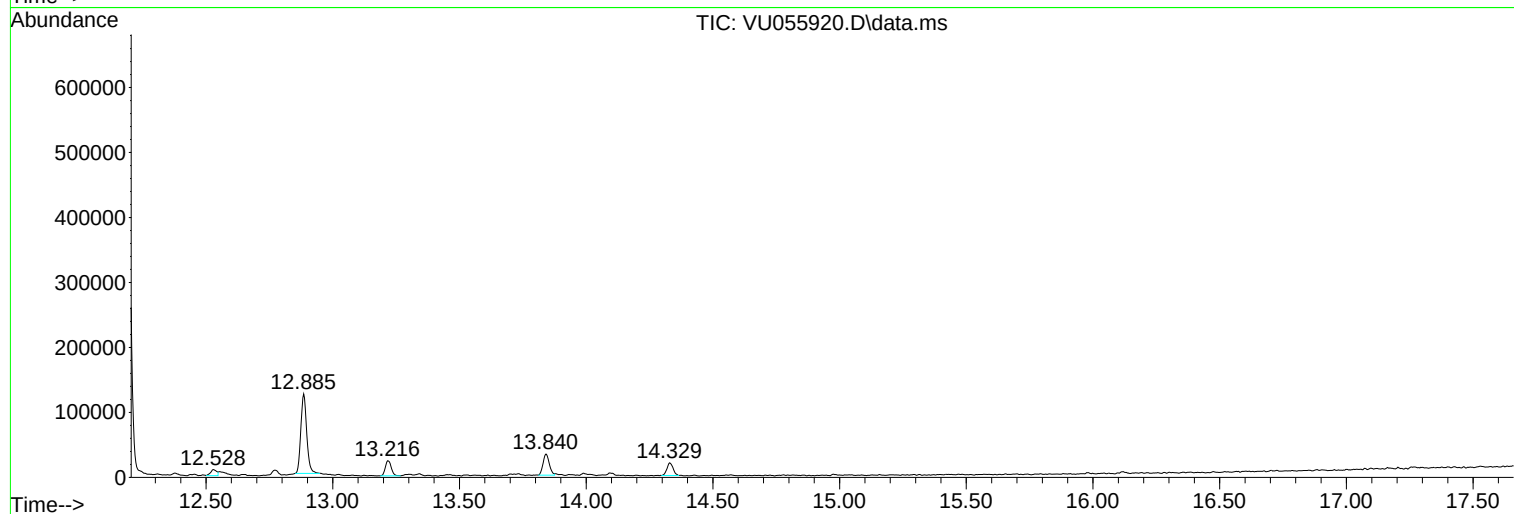
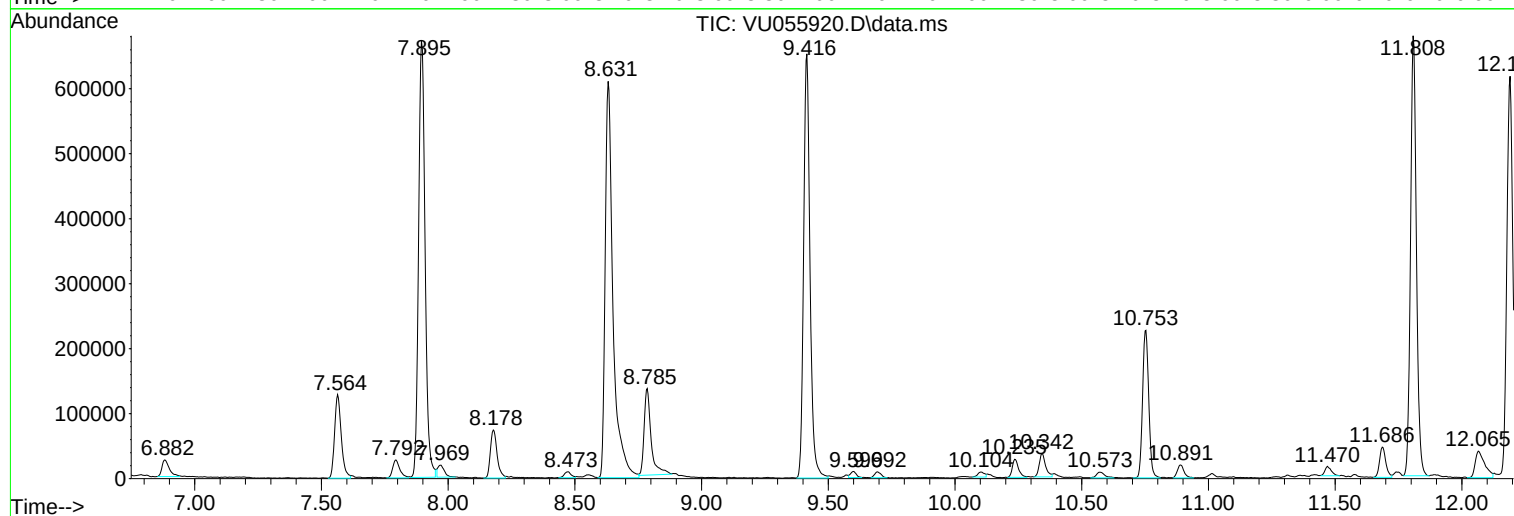
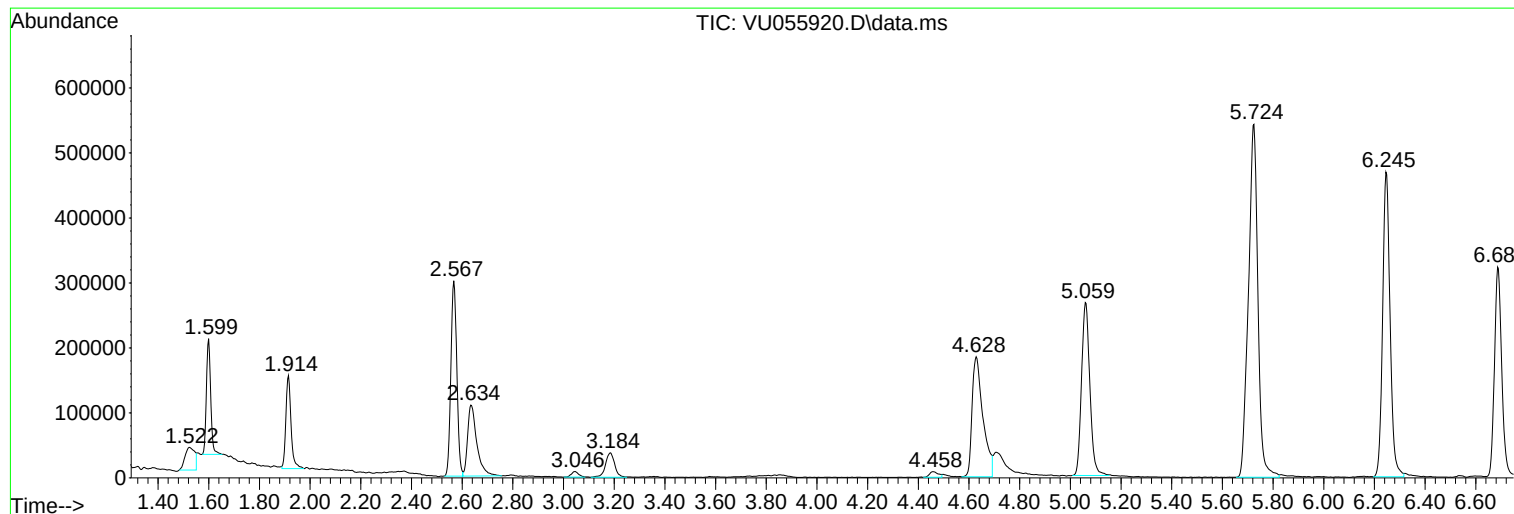
Sum of corrected areas: 13275834

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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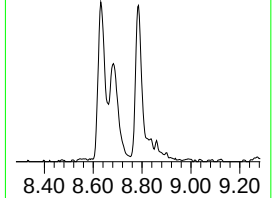
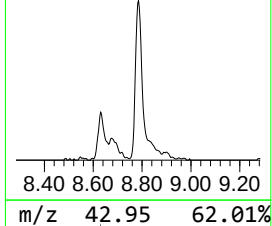
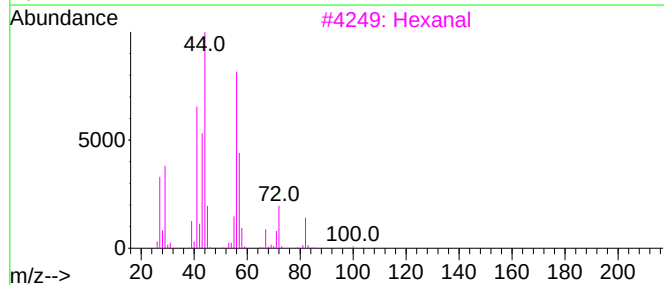
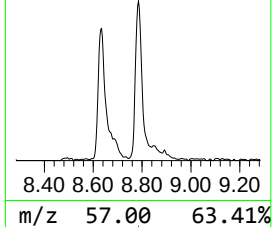
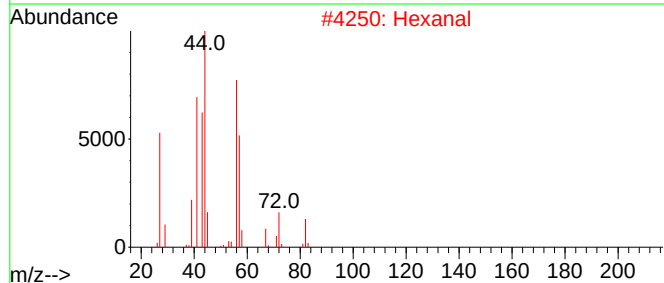
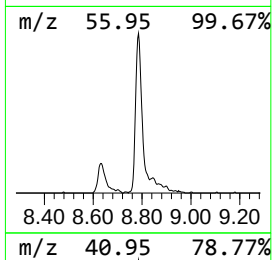
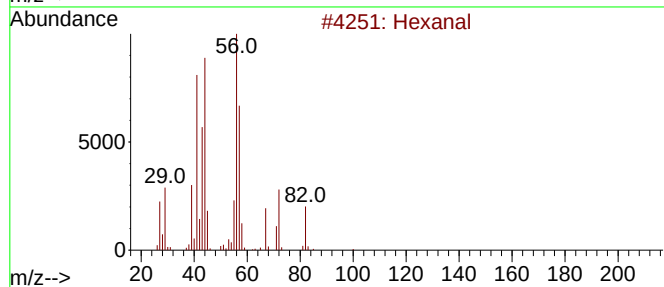
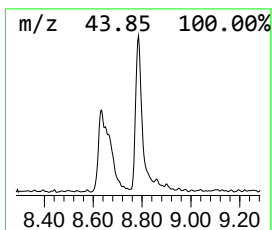
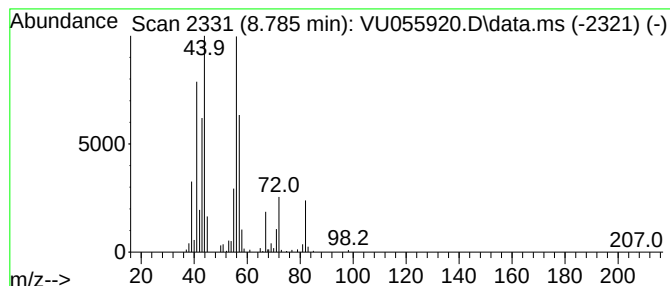
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	1.12 ug/L	258487	Chlorobenzene-d5	9.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	86
2	Hexanal			100	C6H12O	000066-25-1	80
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	53
5	Butanal, 3-methyl-			86	C5H10O	000590-86-3	35



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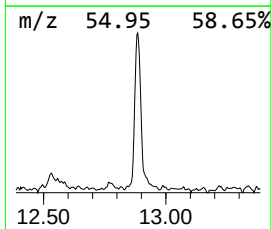
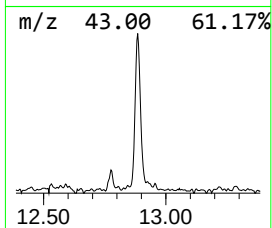
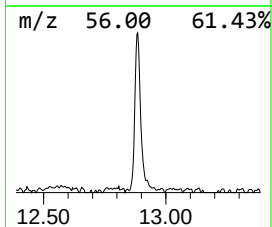
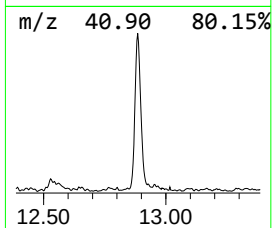
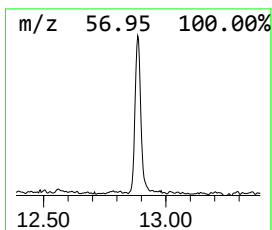
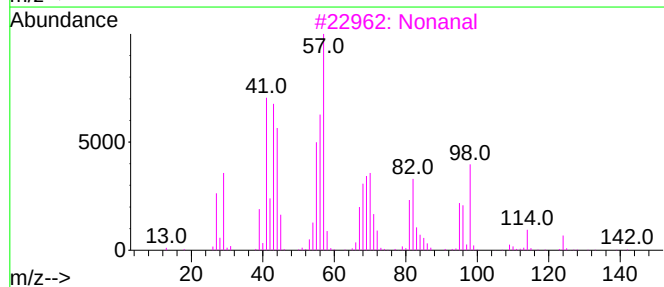
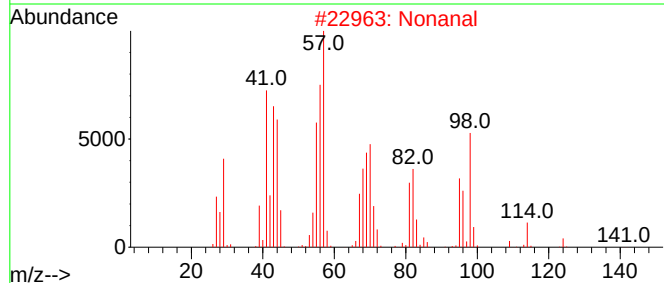
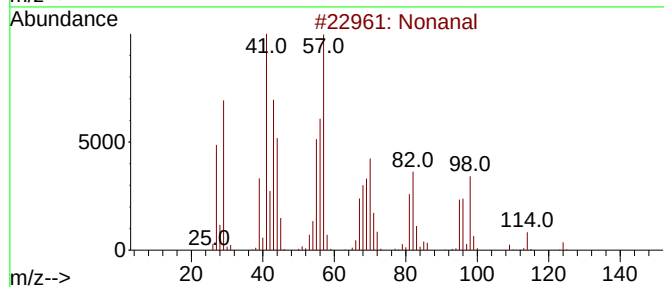
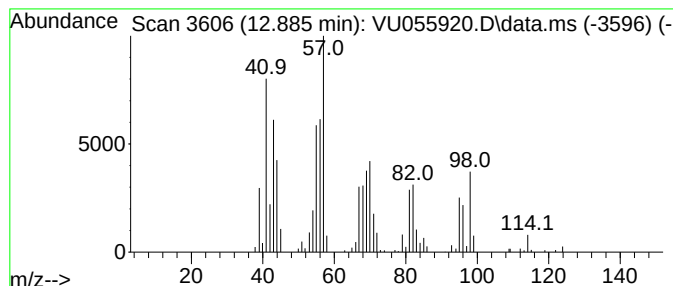
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.885	0.89 ug/L	196927	1,4-Dichlorobenzene-d4	11.808

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	72
4	2-Nonen-1-ol, (E)-			142	C9H18O	031502-14-4	38
5	Cycloheptane			98	C7H14	000291-64-5	38



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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	1.1	ug/L	258487	2	9.416	1151260	5.0
Nonanal	12.885	0.9	ug/L	196927	3	11.808	1102520	5.0