

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU010822\
 Data File : VU046706.D
 Acq On : 08 Jan 2022 15:13
 Operator : SY/MD
 Sample : N1077-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXW2

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\SFAMUTR122121WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU046706.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	17	rVB2	4842	5197	1.13%	0.151%
2	1.604	72	82	96	rVB	38263	46454	10.07%	1.351%
3	1.919	171	180	194	rBV	31256	41497	8.99%	1.207%
4	2.575	369	384	399	rBV	63174	107610	23.32%	3.130%
5	3.369	618	631	645	rVB3	2396	4927	1.07%	0.143%
6	4.658	1014	1032	1081	rBV2	42284	180485	39.12%	5.250%
7	5.067	1143	1159	1180	rBV2	60714	133653	28.97%	3.888%
8	5.729	1344	1365	1392	rBV2	117620	311292	67.47%	9.055%
9	6.250	1513	1527	1545	rVB	100940	190849	41.37%	5.551%
10	6.543	1608	1618	1631	rBB2	18453	32976	7.15%	0.959%
11	6.694	1650	1665	1685	rBV	75536	146325	31.72%	4.256%
12	6.883	1710	1724	1739	rBV3	5471	11655	2.53%	0.339%
13	7.568	1924	1937	1955	rVB	38167	65850	14.27%	1.915%
14	7.899	2027	2040	2055	rBV	141052	241597	52.37%	7.028%
15	7.970	2055	2062	2072	rVB	4144	7249	1.57%	0.211%
16	8.182	2117	2128	2141	rBV	24629	41707	9.04%	1.213%
17	8.472	2209	2218	2231	rBV	2999	5203	1.13%	0.151%
18	8.555	2232	2244	2257	rBV2	87537	145694	31.58%	4.238%
19	8.636	2257	2269	2306	rBV	242517	461360	100.00%	13.420%
20	8.787	2306	2316	2339	rVB	53518	91316	19.79%	2.656%
21	9.417	2499	2512	2531	rBV	159159	265402	57.53%	7.720%
22	10.343	2790	2800	2812	rBV3	9459	14628	3.17%	0.426%
23	10.758	2918	2929	2945	rBV	76651	124530	26.99%	3.622%
24	10.893	2962	2971	2981	rVB2	6274	10120	2.19%	0.294%
25	11.295	3089	3096	3108	rVB4	13101	20288	4.40%	0.590%
26	11.687	3209	3218	3228	rBV2	23791	35026	7.59%	1.019%
27	11.812	3245	3257	3274	rVB	188122	296422	64.25%	8.622%
28	12.063	3328	3335	3344	rBV3	4485	7025	1.52%	0.204%
29	12.192	3364	3375	3389	rBV	159193	255952	55.48%	7.445%
30	12.549	3478	3486	3493	rVB5	4051	5636	1.22%	0.164%
31	12.771	3545	3555	3565	rVB2	5384	7923	1.72%	0.230%
32	12.886	3582	3591	3607	rVB	52191	77771	16.86%	2.262%
33	14.578	4107	4117	4126	rVB2	3789	5644	1.22%	0.164%
34	14.732	4156	4165	4175	rBV3	16947	23231	5.04%	0.676%
35	16.886	4824	4835	4842	rBV4	10240	15339	3.32%	0.446%

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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

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Title : TRACE VOA SFAM1.0

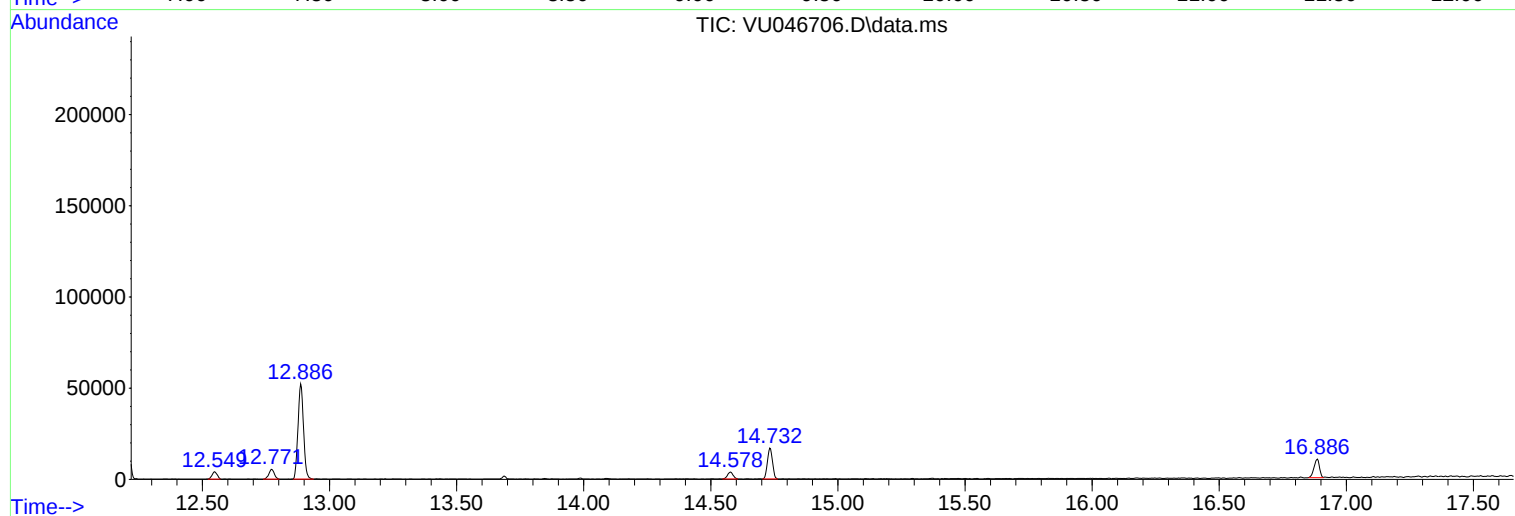
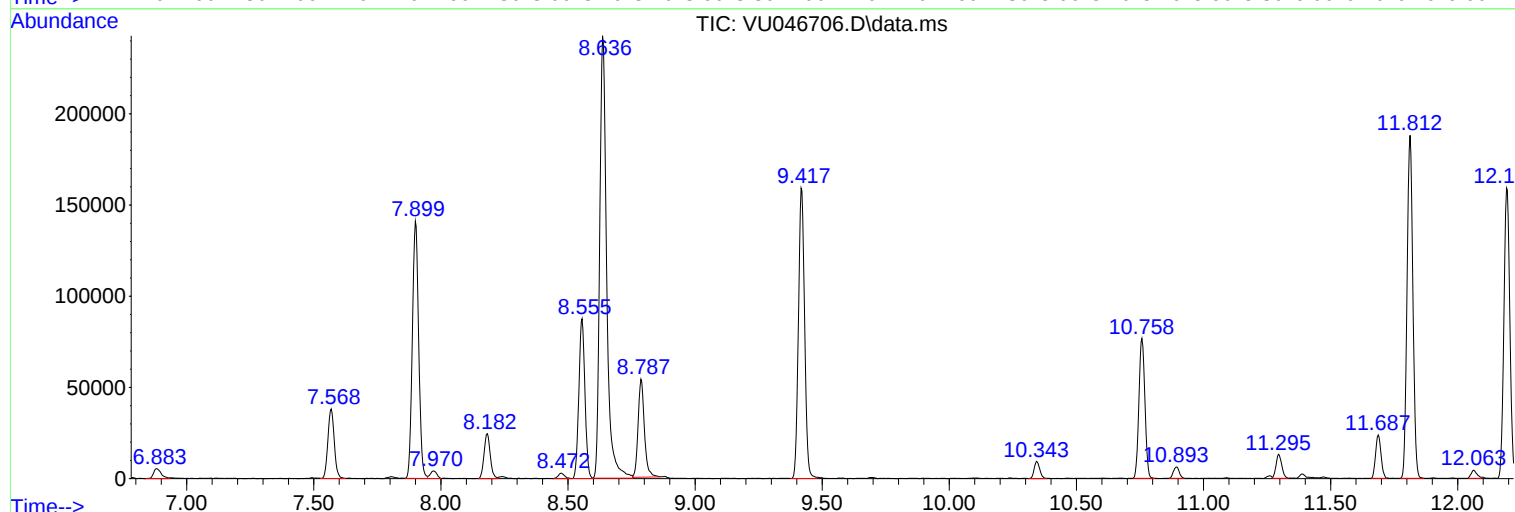
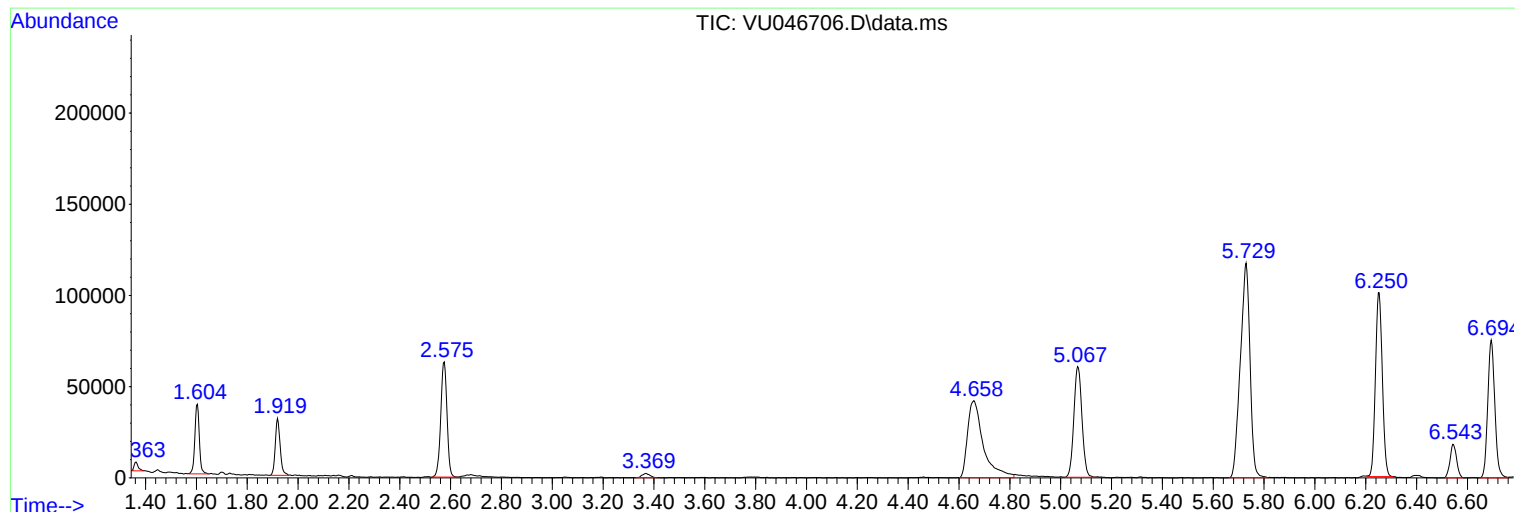
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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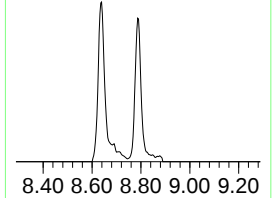
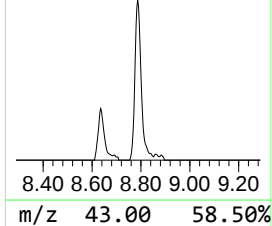
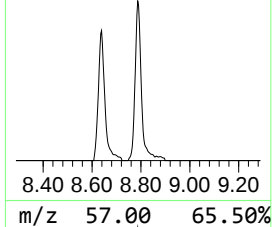
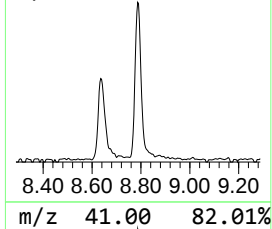
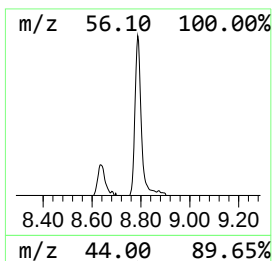
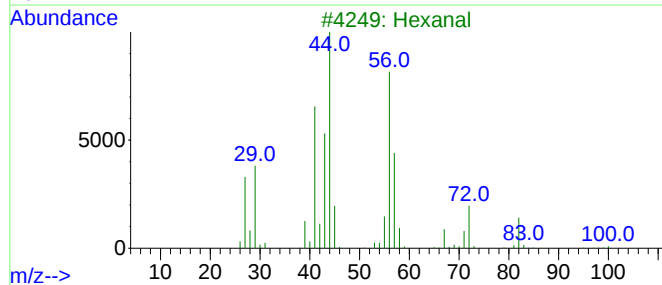
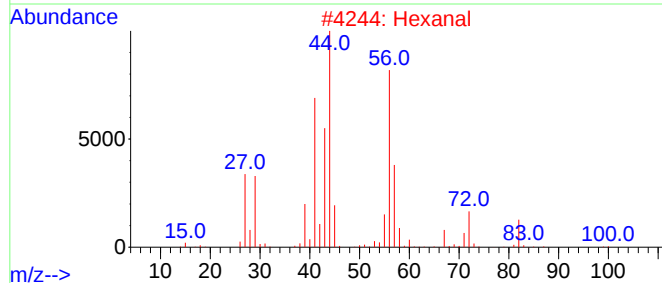
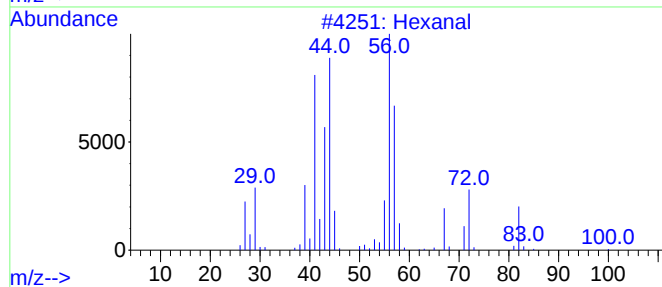
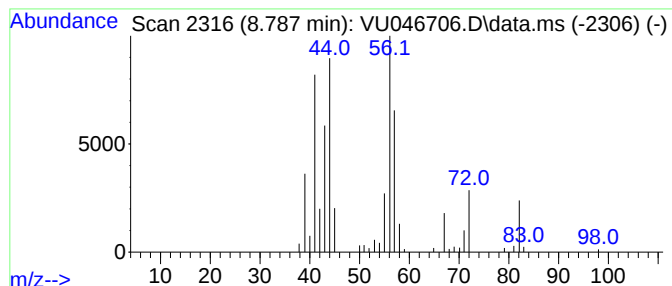
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
8.787	1.72 ug/L	91316	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	83
3	Hexanal			100	C6H12O	000066-25-1	83
4	Hexanal			100	C6H12O	000066-25-1	78
5	Hexanal			100	C6H12O	000066-25-1	72



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW2

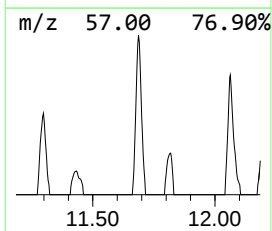
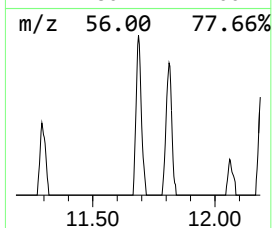
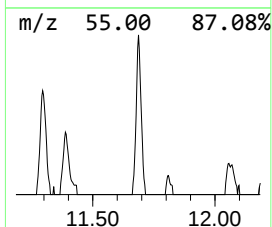
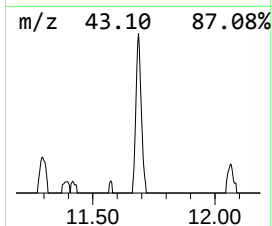
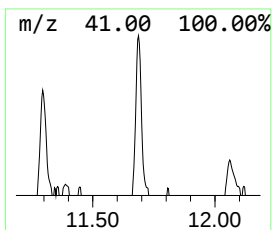
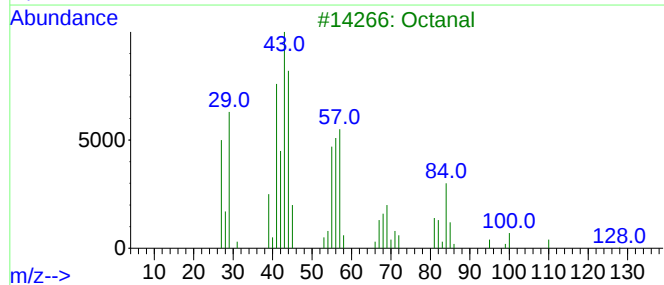
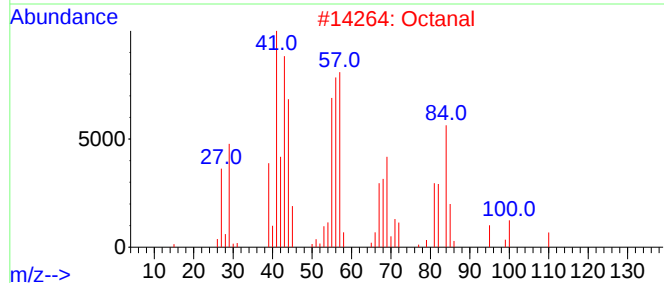
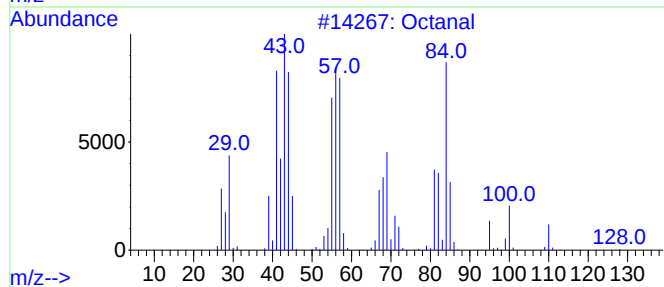
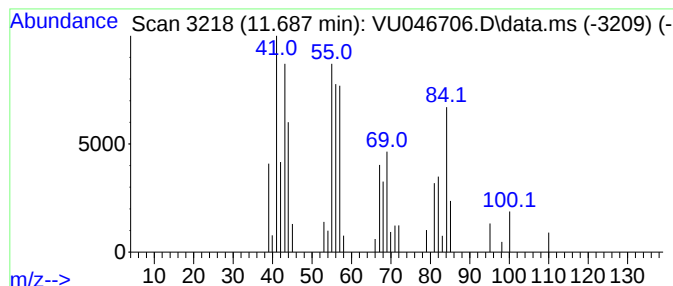
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	0.59 ug/L	35026	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	90
2	Octanal			128	C8H16O	000124-13-0	87
3	Octanal			128	C8H16O	000124-13-0	50
4	Piperazine, 2-methyl-			100	C5H12N2	000109-07-9	43
5	Hydroperoxide, hexyl			118	C6H14O2	004312-76-9	43



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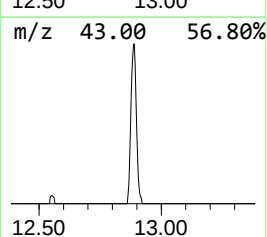
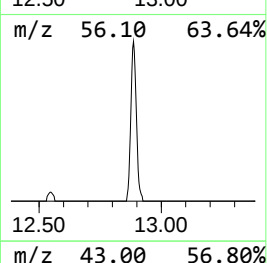
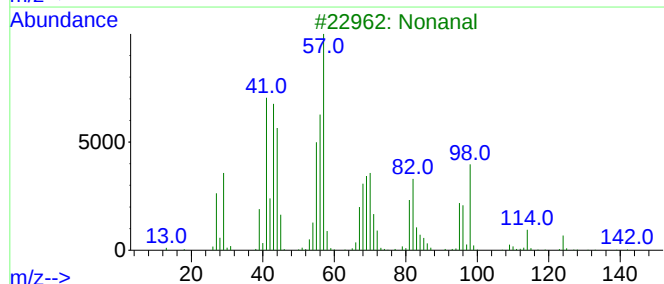
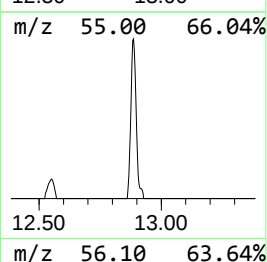
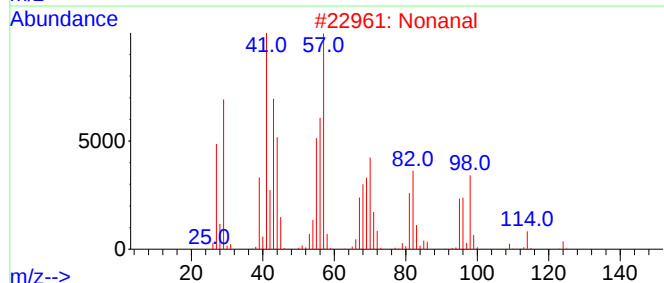
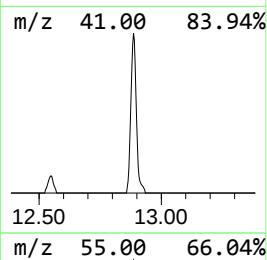
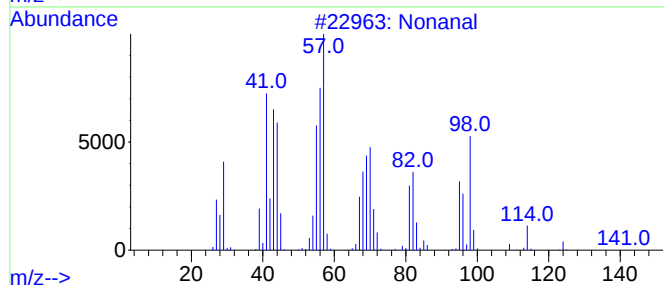
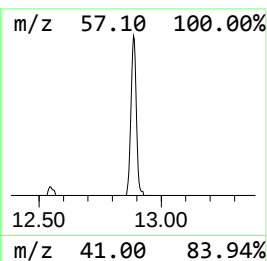
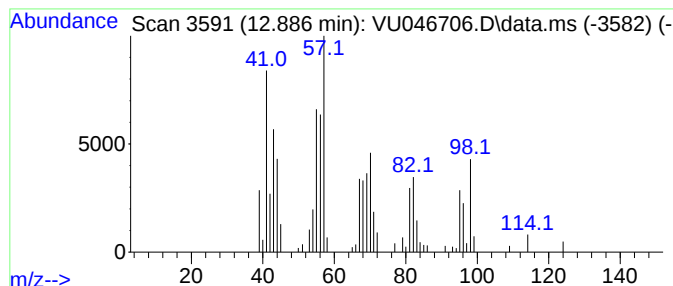
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	1.31 ug/L	77771	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	83
3			Nonanal	142	C9H18O	000124-19-6	80
4			Heptane, 4-chloro-	134	C7H15Cl	000998-95-8	38
5			2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	27



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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	8.787	1.7	ug/L	91316	2	9.420	265402	5.0
Octanal	11.687	0.6	ug/L	35026	3	11.812	296422	5.0
Nonanal	12.886	1.3	ug/L	77771	3	11.812	296422	5.0