

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
 Data File : VU046740.D
 Acq On : 12 Jan 2022 14:16
 Operator : SY/MD
 Sample : N1101-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXW8

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: VU046740.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	71	81	91	rBV	28168	38077	2.32%	0.660%
2	1.919	171	180	198	rVB	22482	30844	1.88%	0.535%
3	2.578	367	385	400	rBV3	66549	135577	8.25%	2.350%
4	4.655	1014	1031	1086	rBV2	33478	173076	10.53%	2.999%
5	5.067	1144	1159	1178	rBV	49779	111914	6.81%	1.939%
6	5.321	1223	1238	1254	rBB2	30677	68109	4.14%	1.180%
7	5.729	1343	1365	1388	rBV3	92262	247538	15.06%	4.290%
8	6.250	1512	1527	1547	rBV	86473	161217	9.81%	2.794%
9	6.693	1652	1665	1684	rBV2	60136	117282	7.14%	2.032%
10	6.880	1710	1723	1744	rBV3	18394	38209	2.32%	0.662%
11	7.568	1924	1937	1957	rVB	32282	53582	3.26%	0.929%
12	7.899	2028	2040	2054	rBV	111969	190479	11.59%	3.301%
13	8.182	2118	2128	2141	rBV2	19760	32499	1.98%	0.563%
14	8.555	2231	2244	2258	rBV	238550	402708	24.50%	6.979%
15	8.639	2258	2270	2297	rVB	212860	404625	24.62%	7.012%
16	8.787	2303	2316	2342	rBV	149266	267356	16.27%	4.633%
17	9.417	2500	2512	2529	rBV	129971	214300	13.04%	3.714%
18	10.343	2789	2800	2821	rBV	75656	125373	7.63%	2.173%
19	10.758	2918	2929	2943	rBV	65728	104950	6.39%	1.819%
20	11.687	3204	3218	3233	rBV	400657	591237	35.97%	10.246%
21	11.812	3244	3257	3273	rVB	163145	258889	15.75%	4.487%
22	12.192	3362	3375	3390	rBV	133201	213158	12.97%	3.694%
23	12.539	3472	3483	3498	rBV3	28790	56485	3.44%	0.979%
24	12.886	3577	3591	3617	rBV	1147028	1643647	100.00%	28.484%
25	14.732	4154	4165	4182	rBV2	47064	71674	4.36%	1.242%
26	16.886	4825	4835	4845	rVB3	11569	17575	1.07%	0.305%

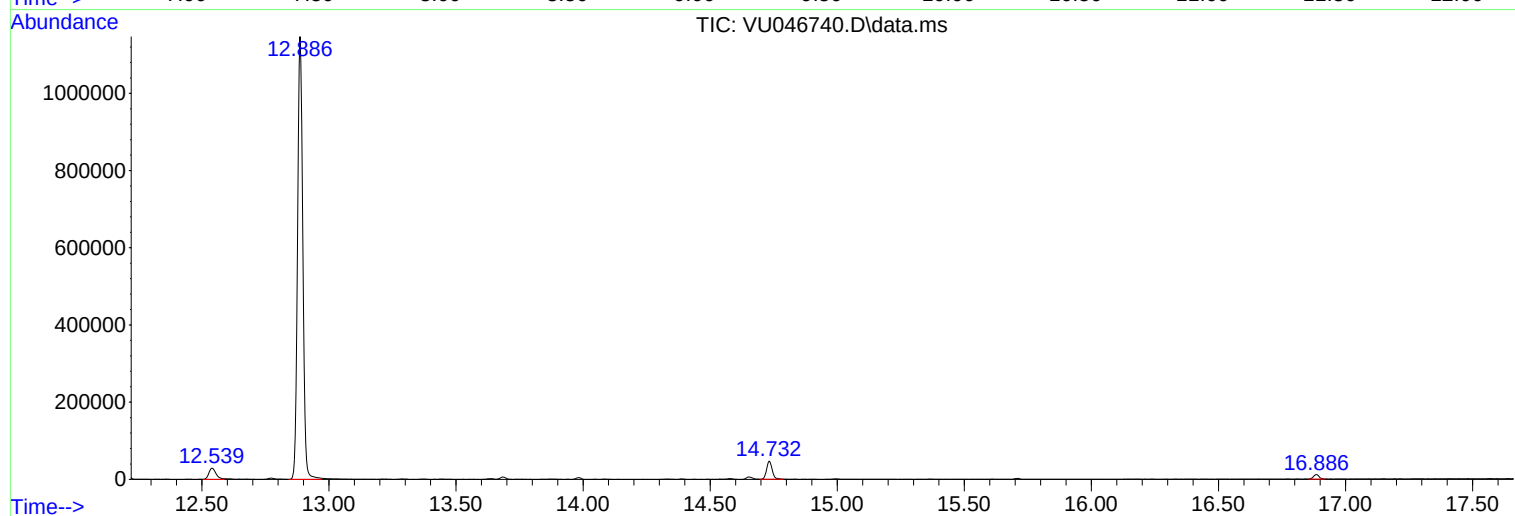
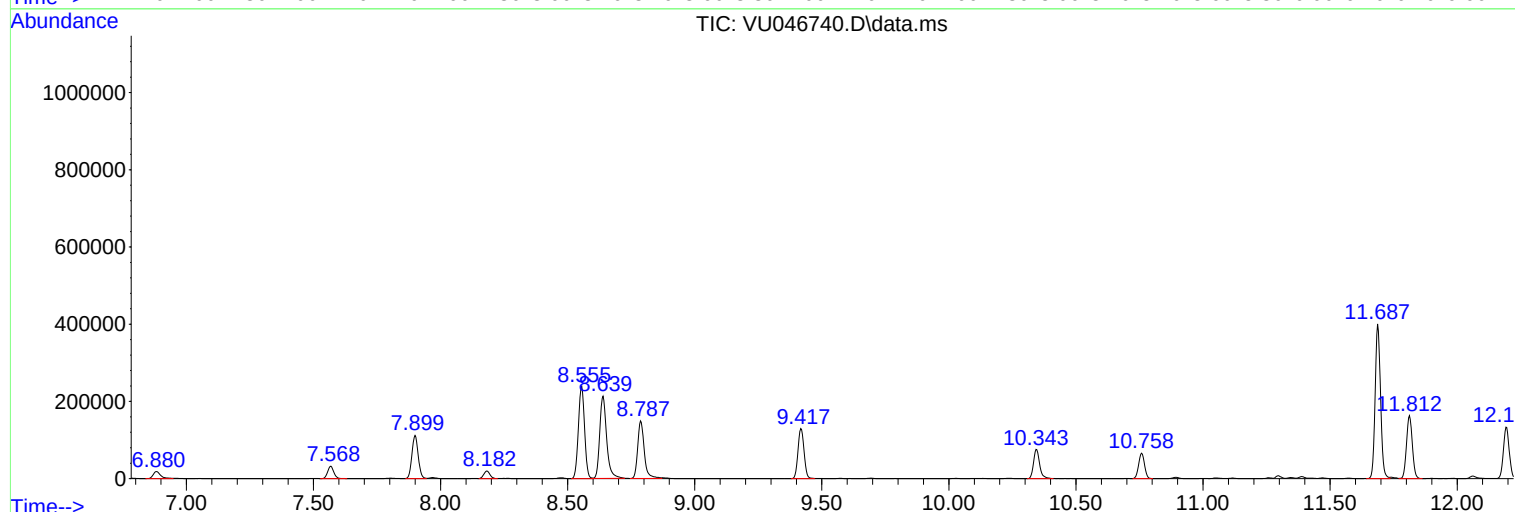
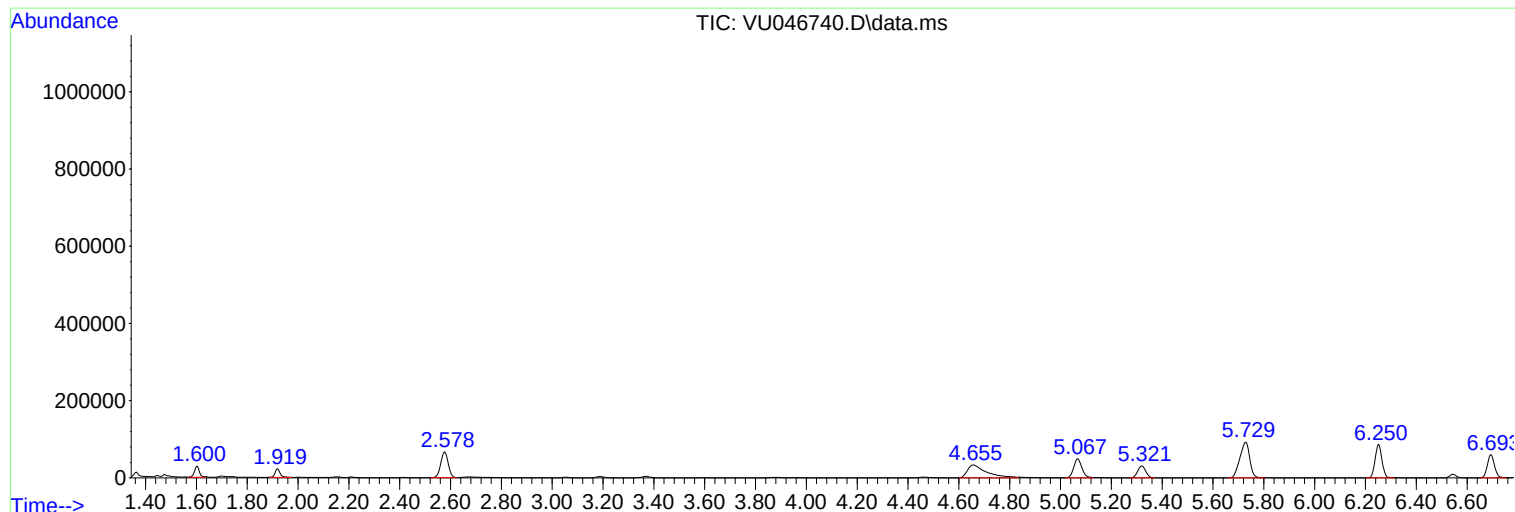
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW8

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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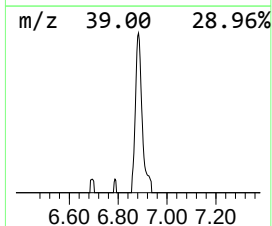
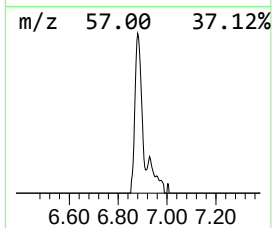
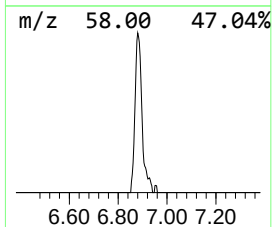
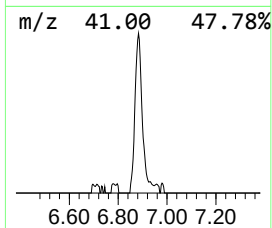
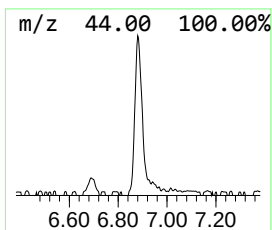
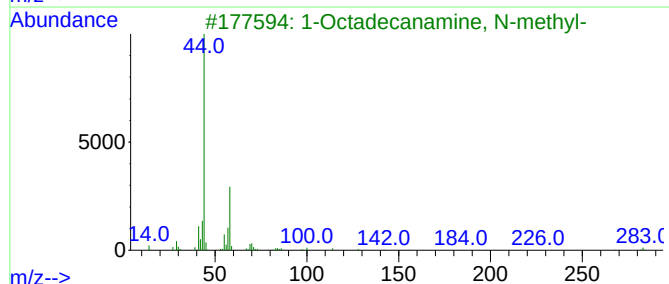
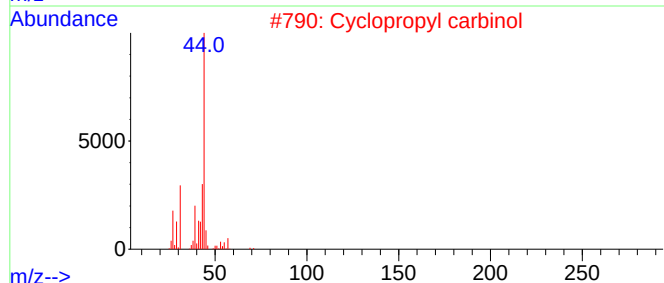
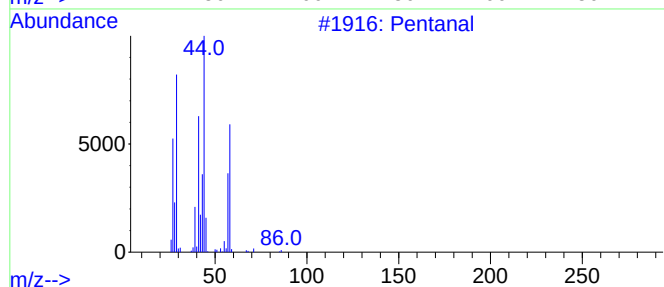
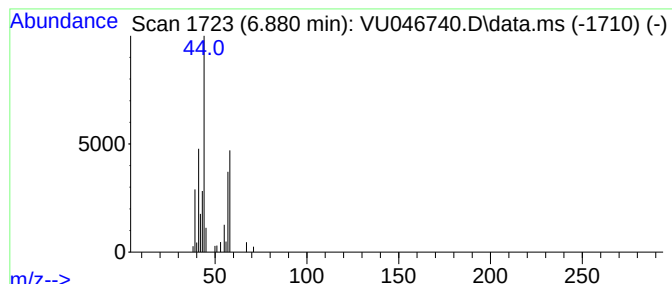
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	1.19 ug/L	38209	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	78
2			Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
3			1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	9
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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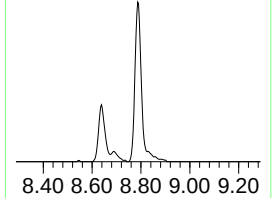
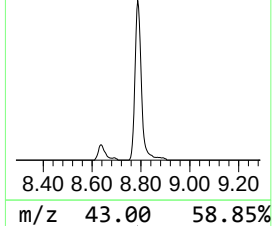
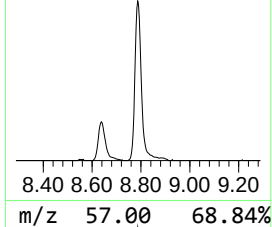
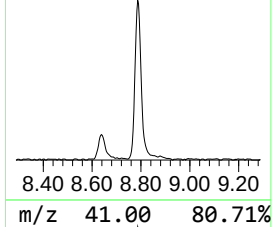
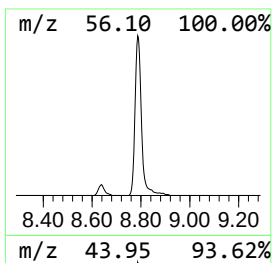
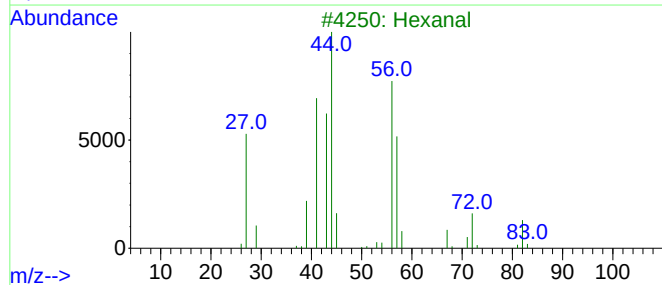
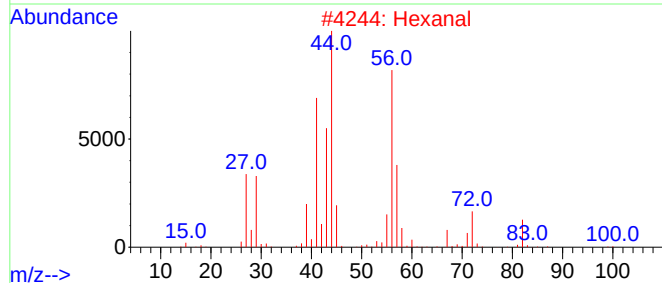
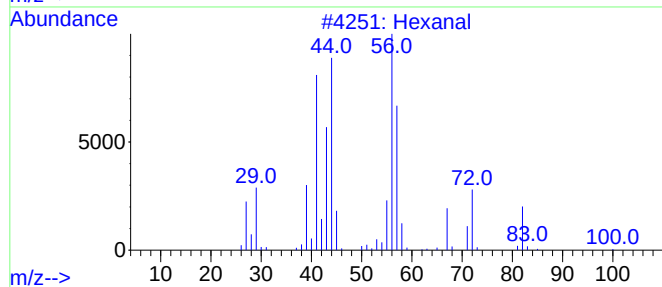
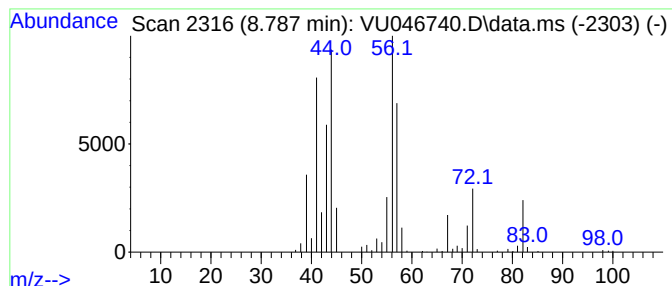
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	6.24 ug/L	267356	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	96
2	Hexanal			100	C6H12O	000066-25-1	91
3	Hexanal			100	C6H12O	000066-25-1	83
4	Hexanal			100	C6H12O	000066-25-1	83
5	Hexanal			100	C6H12O	000066-25-1	83



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

Instrument :
MSVOA_U
ClientSampleId :
BFXW8

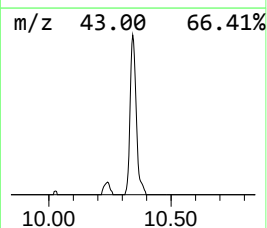
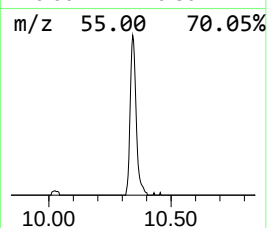
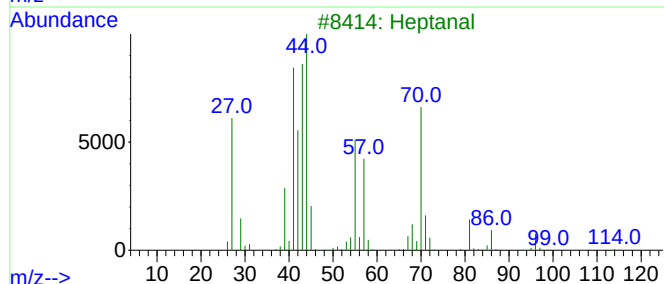
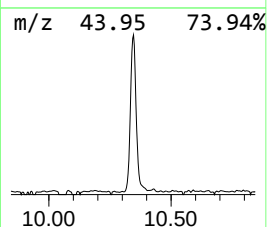
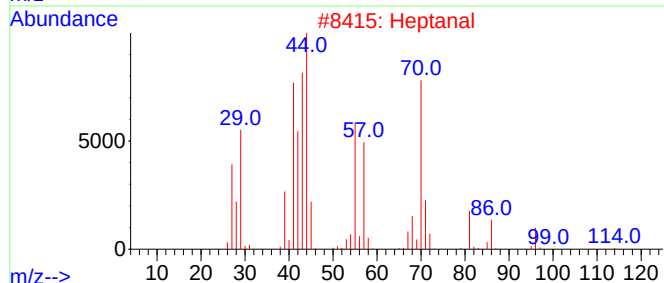
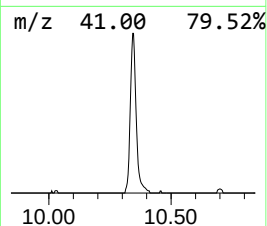
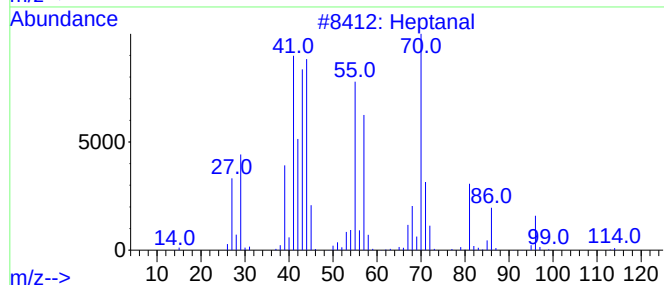
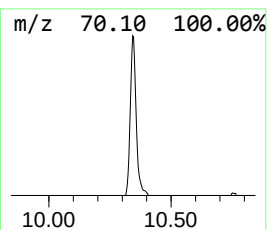
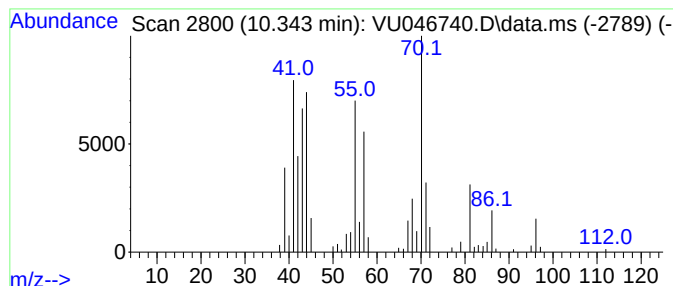
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.343	2.93 ug/L	125373	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	91
2			Heptanal	114	C7H14O	000111-71-7	72
3			Heptanal	114	C7H14O	000111-71-7	72
4			Heptanal	114	C7H14O	000111-71-7	72
5			Heptanal	114	C7H14O	000111-71-7	59



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ALS Vial : 9 Sample Multiplier: 1

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ClientSampleId :
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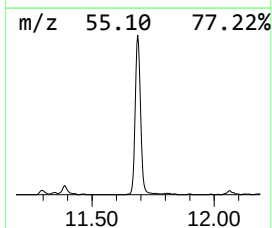
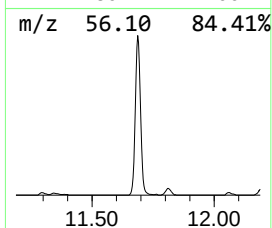
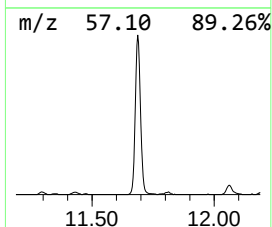
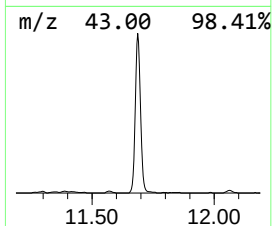
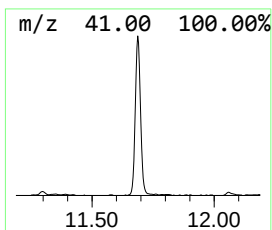
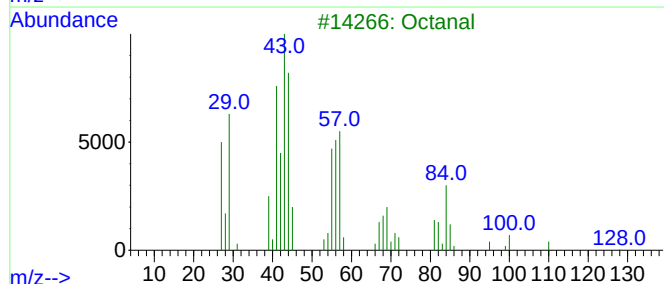
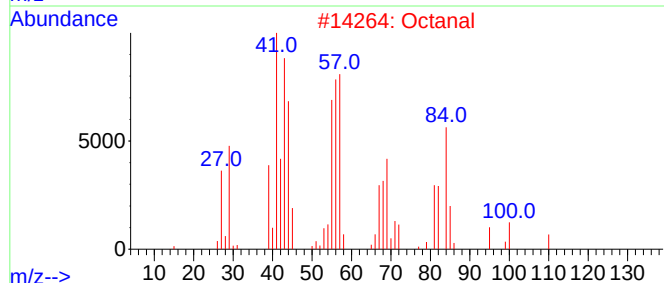
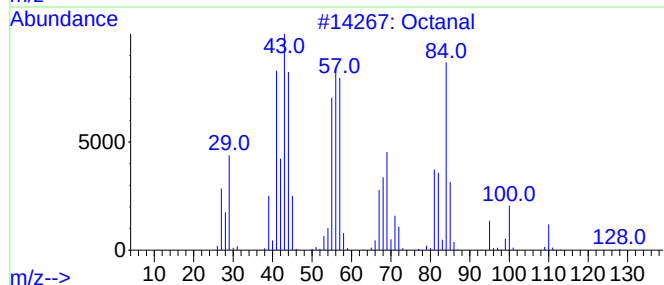
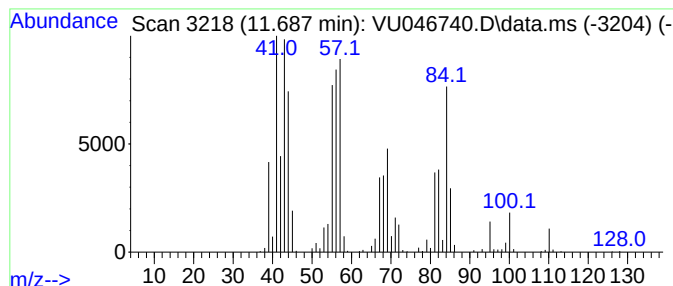
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	11.42 ug/L	591237	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	98
2	Octanal			128	C8H16O	000124-13-0	91
3	Octanal			128	C8H16O	000124-13-0	90
4	Octanal			128	C8H16O	000124-13-0	76
5	Octanal			128	C8H16O	000124-13-0	76



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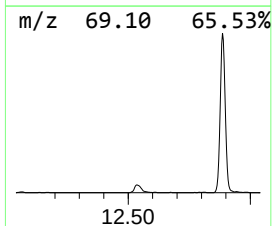
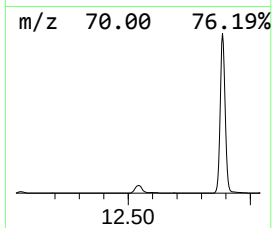
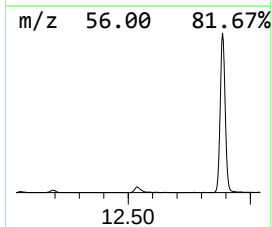
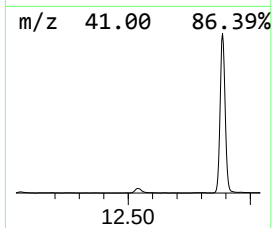
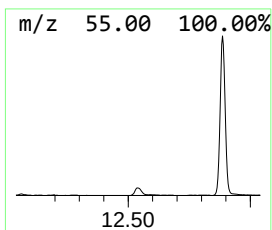
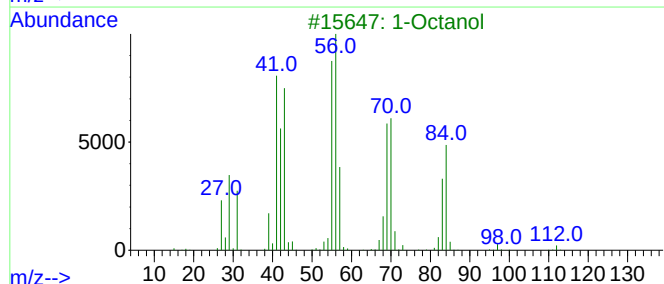
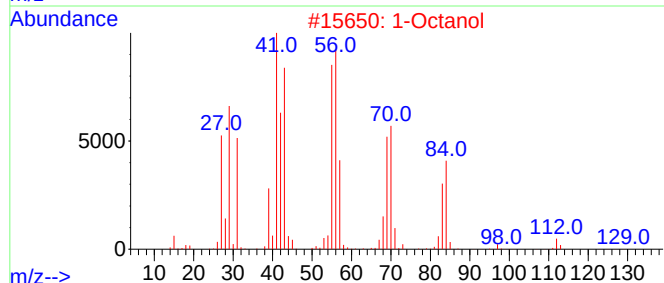
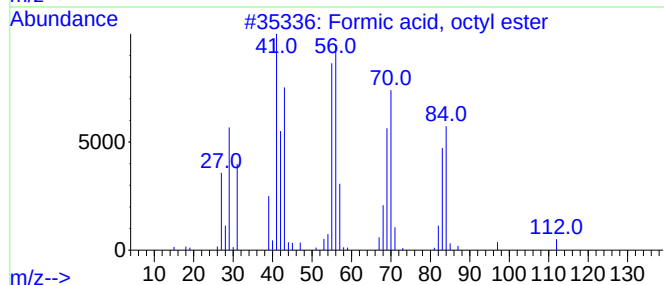
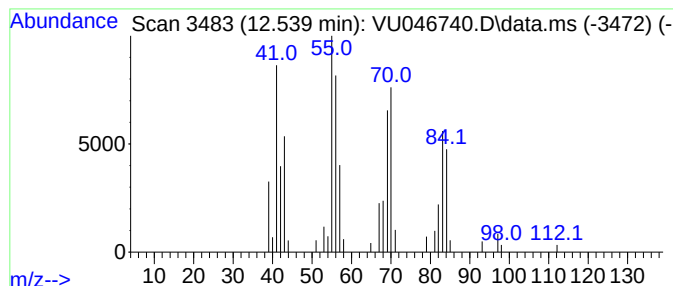
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Formic acid, octyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.539	1.09 ug/L	56485	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formic acid, octyl ester	158	C9H18O2	000112-32-3	78
2			1-Octanol	130	C8H18O	000111-87-5	64
3			1-Octanol	130	C8H18O	000111-87-5	64
4			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	53
5			1,2-Cyclohexanedione	112	C6H8O2	000765-87-7	50



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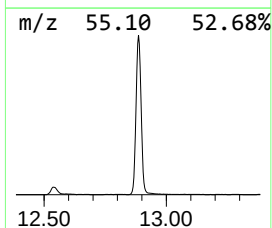
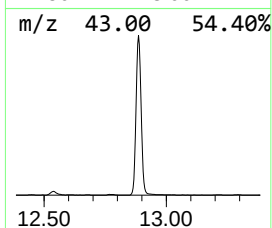
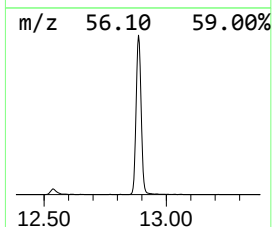
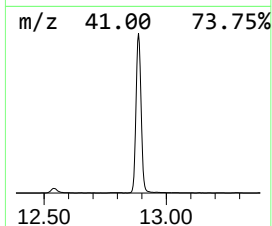
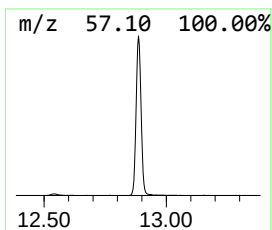
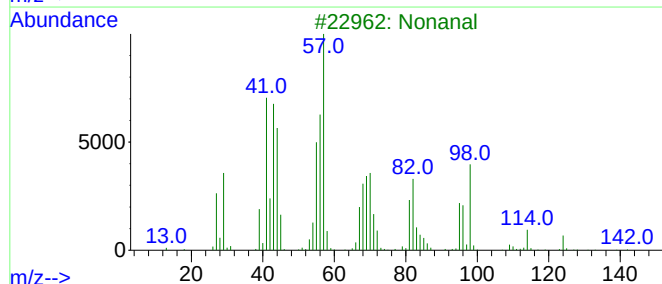
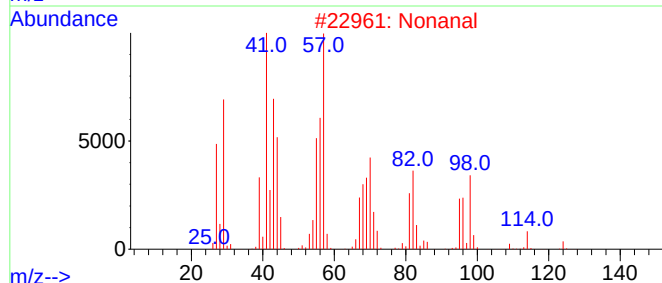
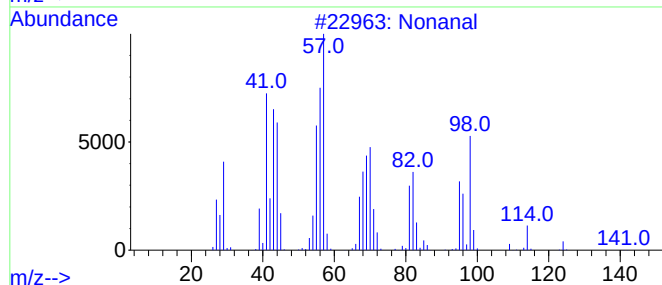
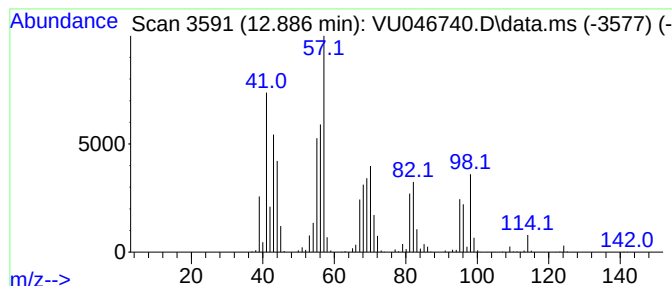
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	31.74 ug/L	1643650	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	91
3			Nonanal	142	C9H18O	000124-19-6	86
4			Nonanal	142	C9H18O	000124-19-6	83
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046740.D
Acq On : 12 Jan 2022 14:16
Operator : SY/MD
Sample : N1101-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW8

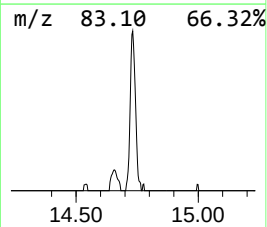
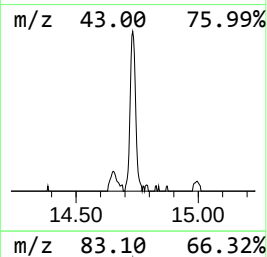
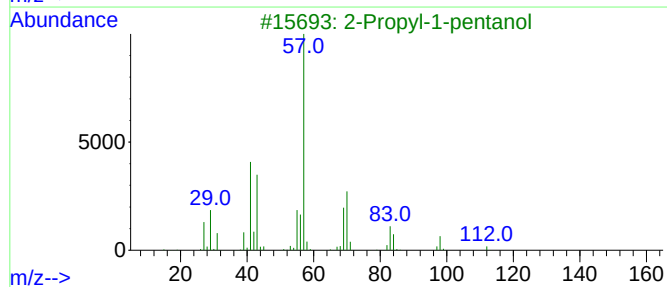
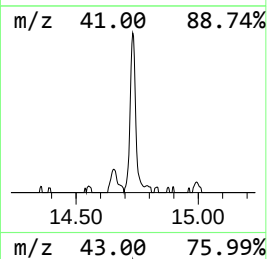
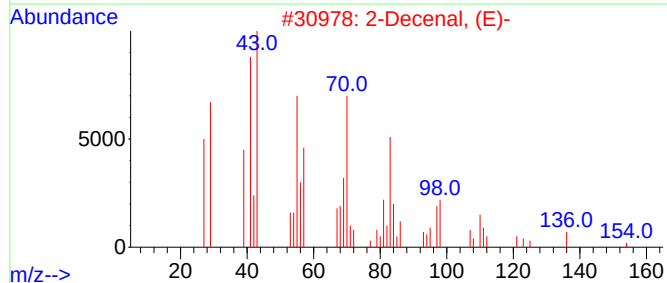
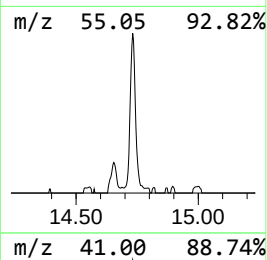
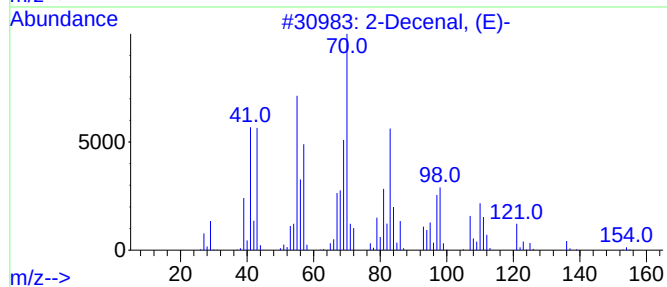
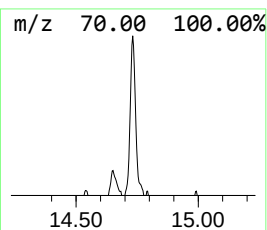
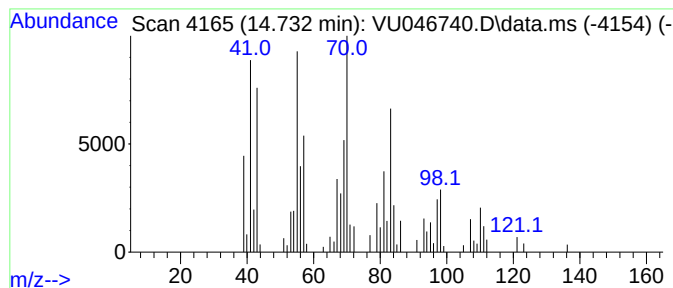
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 2-Decenal, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.732	1.38 ug/L	71674	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decenal, (E)-	154	C10H18O	003913-81-3	74
2			2-Decenal, (E)-	154	C10H18O	003913-81-3	72
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	46
5			Bicyclo[3.1.0]hexan-2-ol	98	C6H10O	1000194-18-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046740.D
Acq On : 12 Jan 2022 14:16
Operator : SY/MD
Sample : N1101-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW8

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	6.880	1.2	ug/L	38209	1	6.250	161217	5.0
Hexanal	8.787	6.2	ug/L	267356	2	9.417	214300	5.0
Heptanal	10.343	2.9	ug/L	125373	2	9.417	214300	5.0
Octanal	11.687	11.4	ug/L	591237	3	11.812	258889	5.0
Formic acid, oc...	12.539	1.1	ug/L	56485	3	11.812	258889	5.0
Nonanal	12.886	31.7	ug/L	1643650	3	11.812	258889	5.0
2-Decenal, (E)-	14.732	1.4	ug/L	71674	3	11.812	258889	5.0