

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012622\
 Data File : VU046847.D
 Acq On : 26 Jan 2022 15:49
 Operator : SY/MD
 Sample : N1260-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX9

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\SFAMUTR011822WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU046847.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	14	rVB	24362	22221	1.35%	0.246%
2	1.475	36	42	46	rBV	26008	27551	1.68%	0.305%
3	1.604	71	82	97	rBV	59165	77465	4.72%	0.856%
4	1.919	172	180	192	rBV	43917	57939	3.53%	0.641%
5	2.585	366	387	403	rBV4	376353	701710	42.75%	7.757%
6	3.366	613	630	654	rBV	122541	287705	17.53%	3.181%
7	3.877	764	789	809	rVB	111893	263375	16.04%	2.912%
8	4.671	1013	1036	1071	rBV2	529239	1322462	80.56%	14.620%
9	5.070	1143	1160	1188	rBV2	81871	203232	12.38%	2.247%
10	5.321	1223	1238	1254	rBV	67555	150874	9.19%	1.668%
11	5.729	1344	1365	1380	rBV2	153914	400863	24.42%	4.432%
12	6.253	1513	1528	1547	rBV	120320	228275	13.91%	2.524%
13	6.546	1604	1619	1651	rBV	877285	1641609	100.00%	18.148%
14	6.694	1652	1665	1684	rVB2	98406	195648	11.92%	2.163%
15	6.880	1714	1723	1740	rBV	21240	41514	2.53%	0.459%
16	7.568	1925	1937	1950	rBV	47362	80215	4.89%	0.887%
17	7.899	2026	2040	2056	rBV	179408	316334	19.27%	3.497%
18	8.182	2116	2128	2142	rBV	28699	48020	2.93%	0.531%
19	8.555	2231	2244	2258	rBV	461725	783288	47.71%	8.659%
20	8.636	2258	2269	2296	rVB	280581	491747	29.96%	5.436%
21	8.787	2304	2316	2344	rBV	175346	305529	18.61%	3.378%
22	9.420	2500	2513	2536	rBV	186509	314536	19.16%	3.477%
23	10.343	2791	2800	2821	rVB3	31141	50252	3.06%	0.556%
24	10.758	2918	2929	2943	rBV	85865	135144	8.23%	1.494%
25	11.687	3208	3218	3229	rBV3	49771	76394	4.65%	0.845%
26	11.812	3245	3257	3278	rVB	213696	341679	20.81%	3.777%
27	12.195	3363	3376	3391	rBV	181130	296957	18.09%	3.283%
28	12.886	3576	3591	3612	rBV	105904	160783	9.79%	1.777%
29	14.732	4157	4165	4174	rBV4	15780	22412	1.37%	0.248%

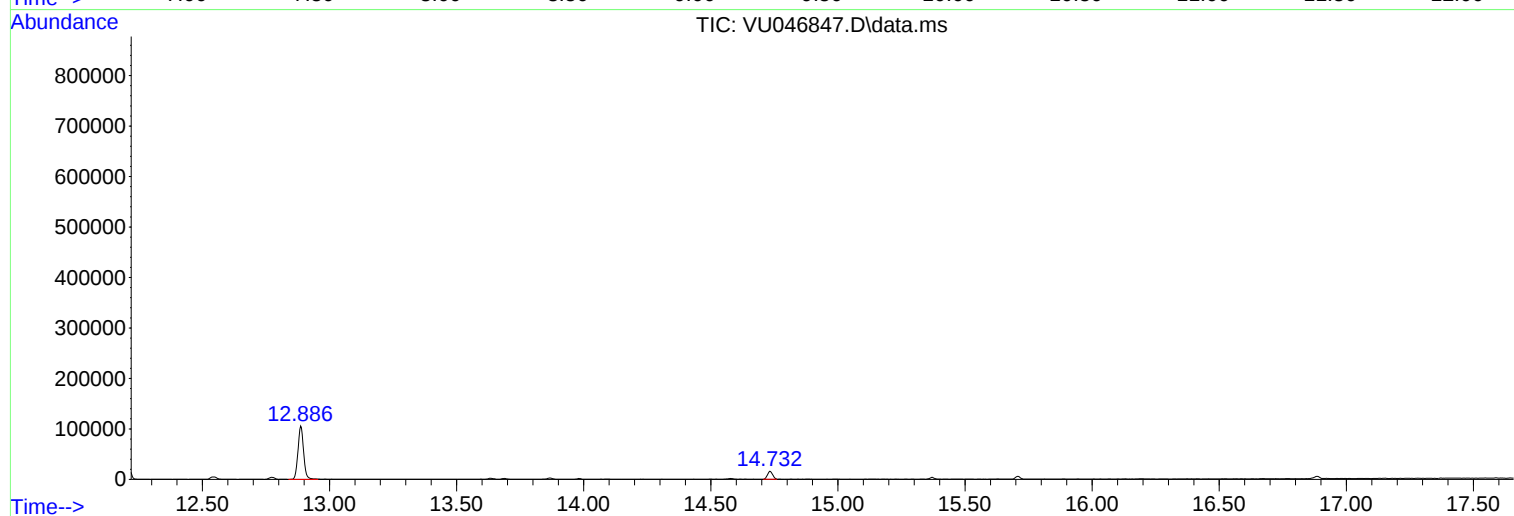
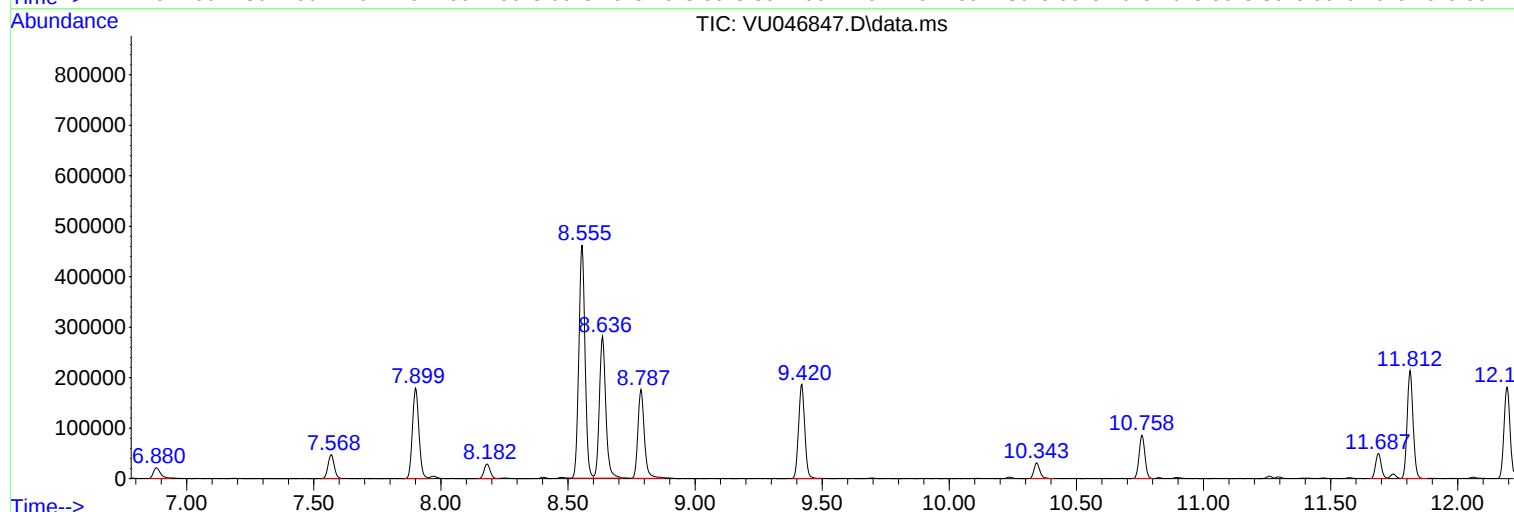
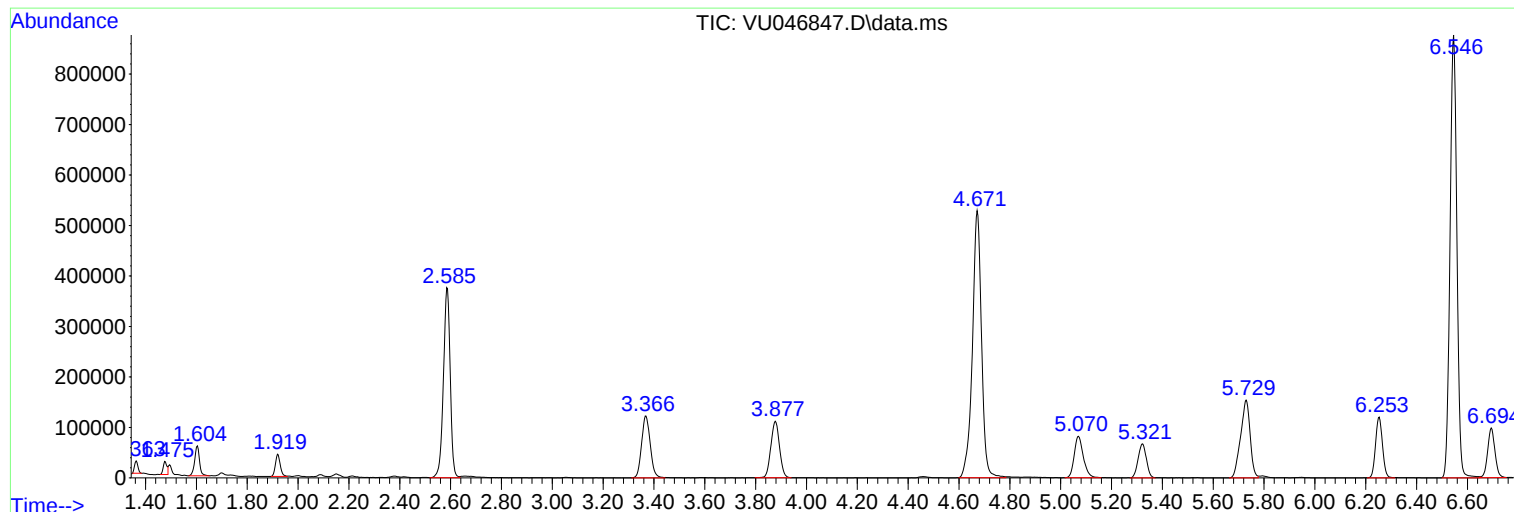
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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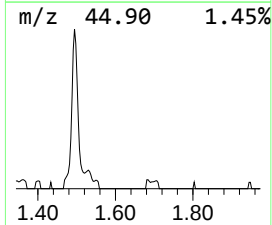
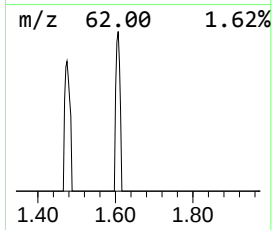
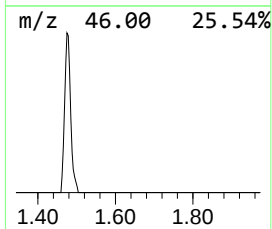
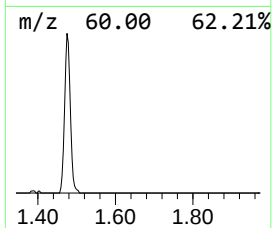
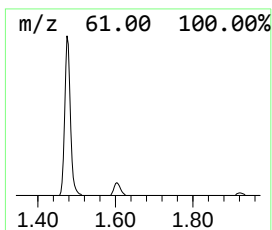
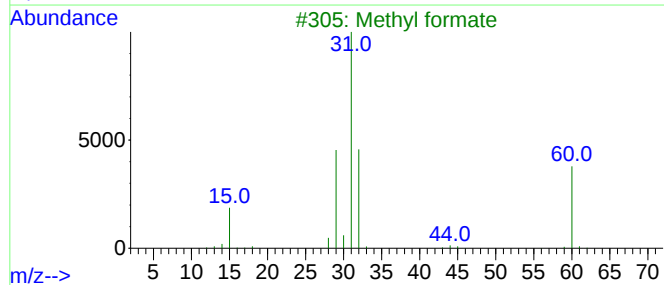
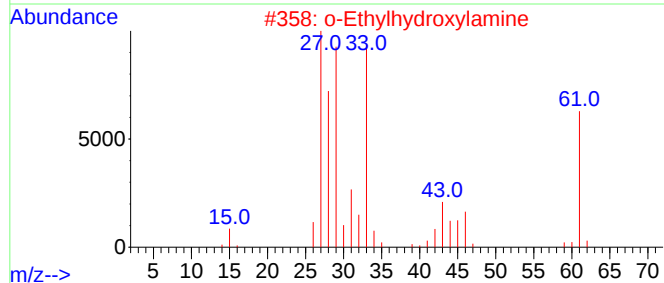
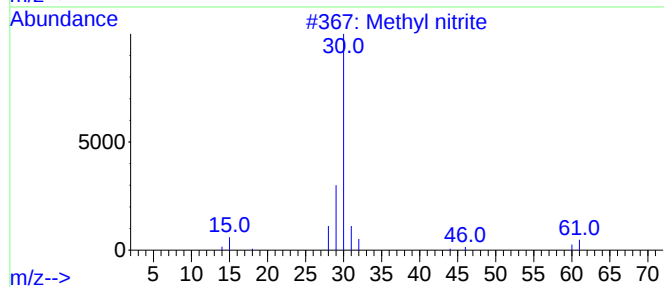
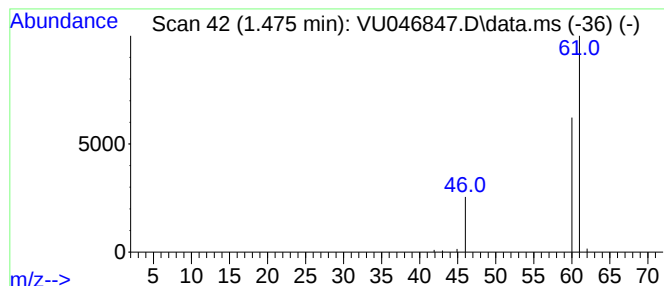
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	0.60 ug/L	27551	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl nitrite	61	CH3NO2	000624-91-9	5
2			o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
3			Methyl formate	60	C2H4O2	000107-31-3	3
4			Urea	60	CH4N2O	000057-13-6	3
5			Urea	60	CH4N2O	000057-13-6	3



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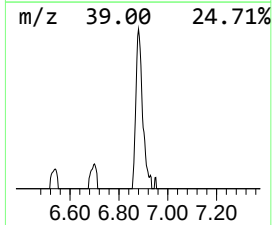
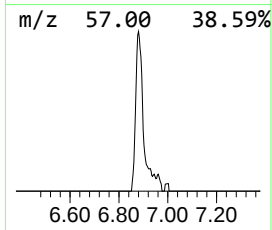
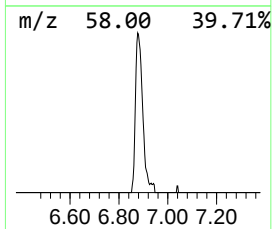
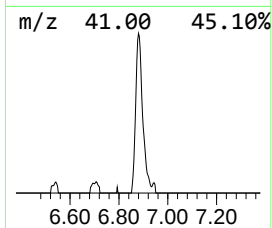
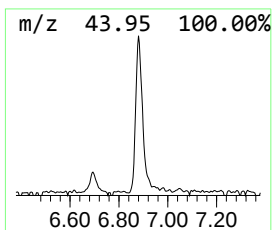
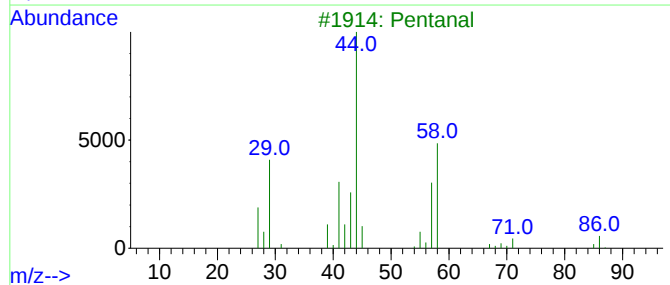
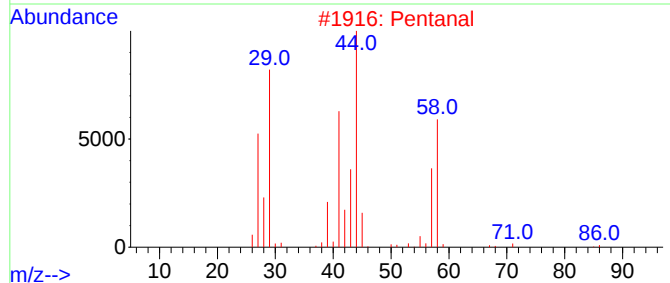
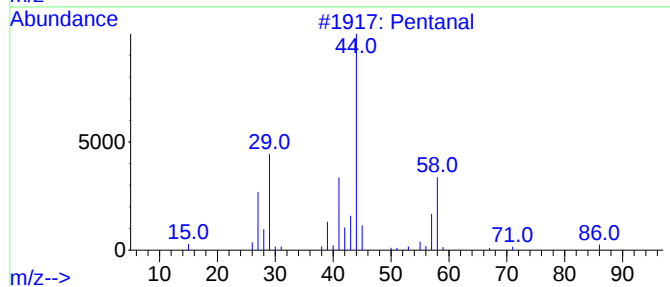
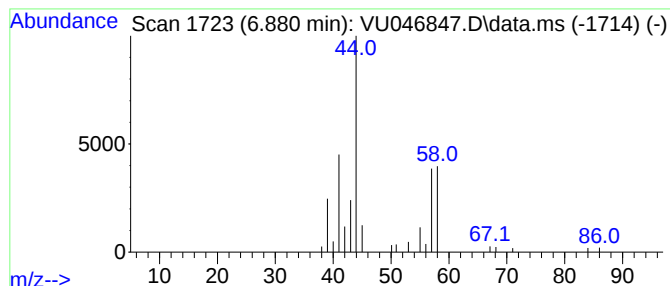
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	0.91 ug/L	41514	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	78
2	Pentanal			86	C5H10O	000110-62-3	56
3	Pentanal			86	C5H10O	000110-62-3	33
4	Butanal, 3-methyl-			86	C5H10O	000590-86-3	25
5	Butanal, 2-methyl-			86	C5H10O	000096-17-3	9



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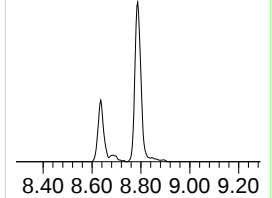
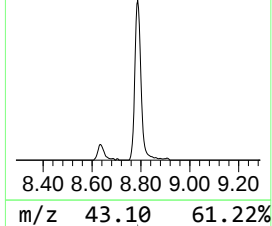
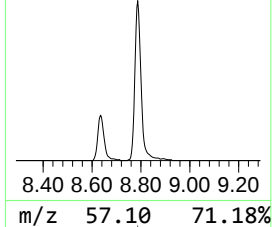
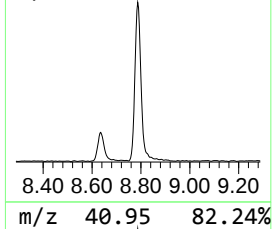
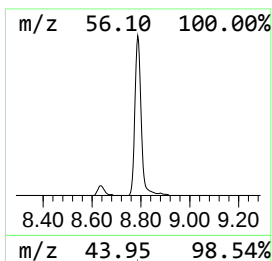
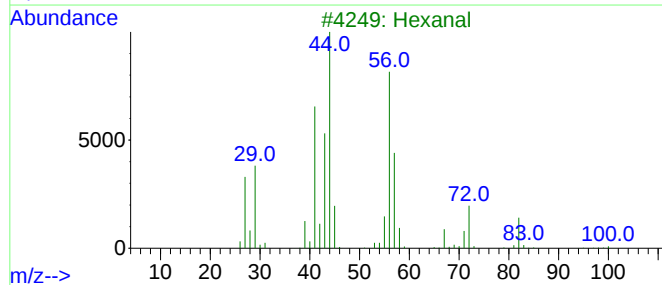
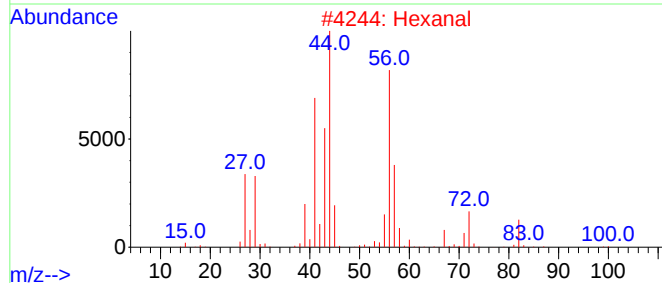
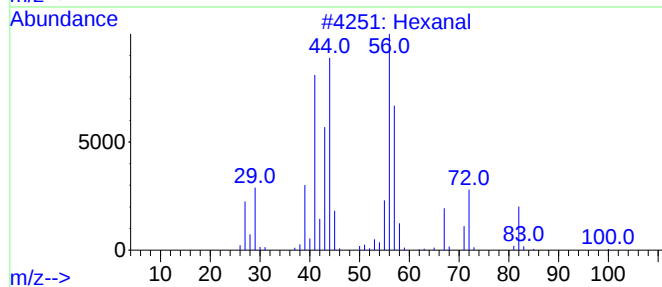
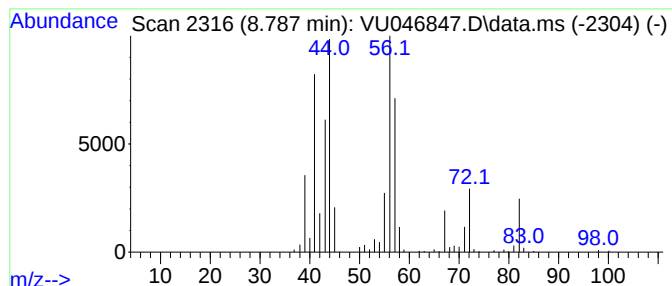
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	4.86 ug/L	305529	Chlorobenzene-d5	9.420

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	91
4	Hexanal			100	C6H12O	000066-25-1	86
5	Hexanal			100	C6H12O	000066-25-1	72



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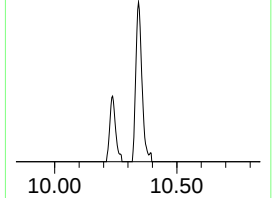
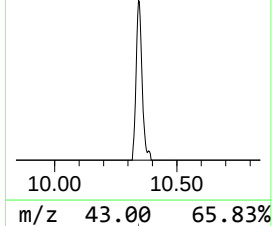
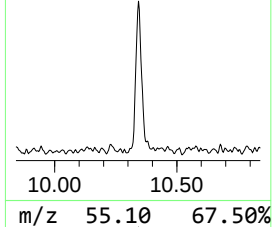
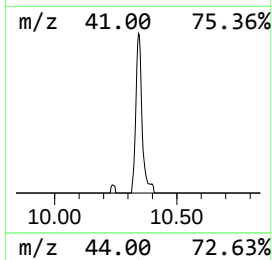
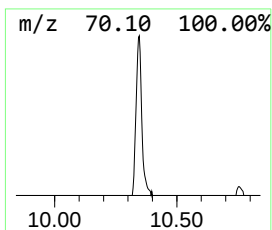
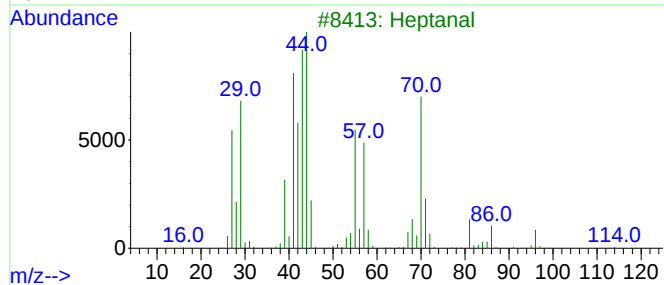
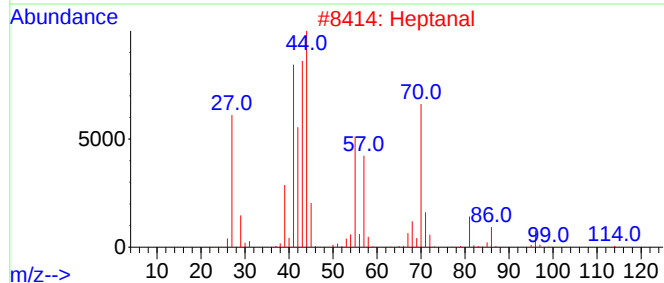
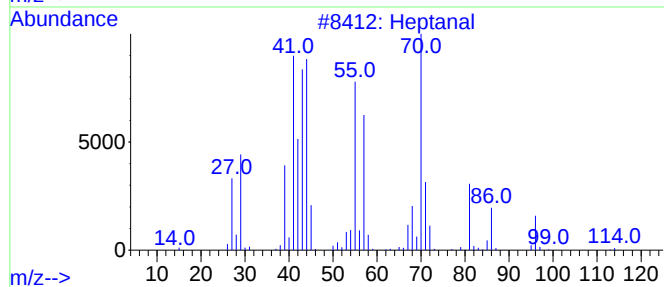
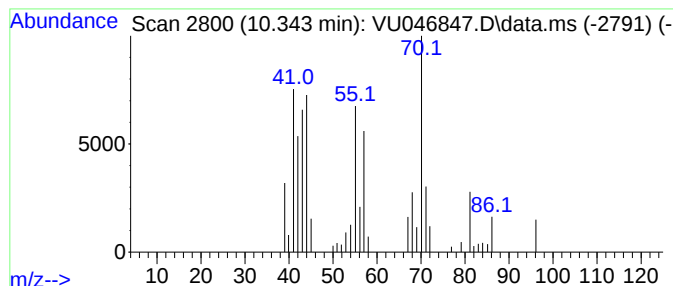
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.343	0.80 ug/L	50252	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	83
2			Heptanal	114	C7H14O	000111-71-7	72
3			Heptanal	114	C7H14O	000111-71-7	59
4			Heptanal	114	C7H14O	000111-71-7	59
5			Heptanal	114	C7H14O	000111-71-7	53



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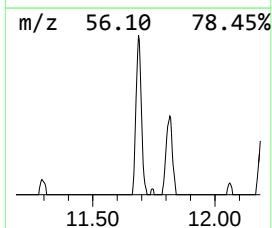
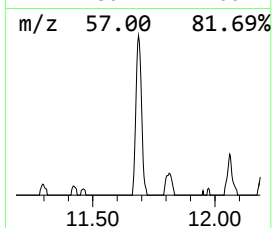
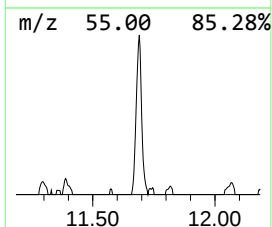
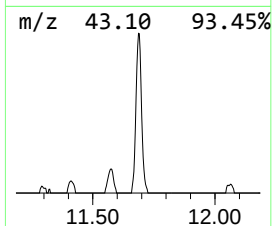
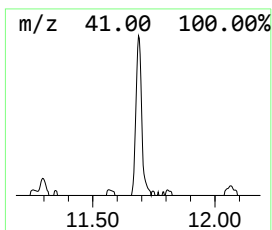
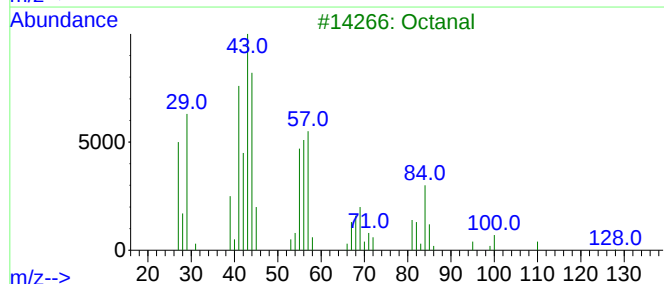
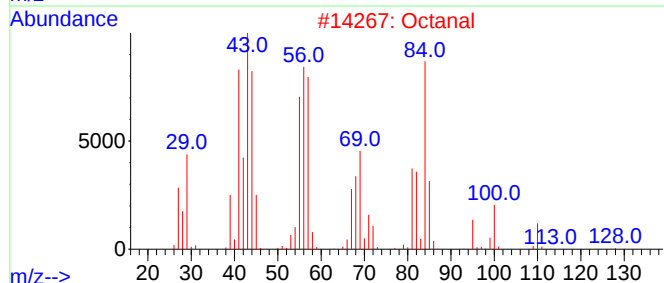
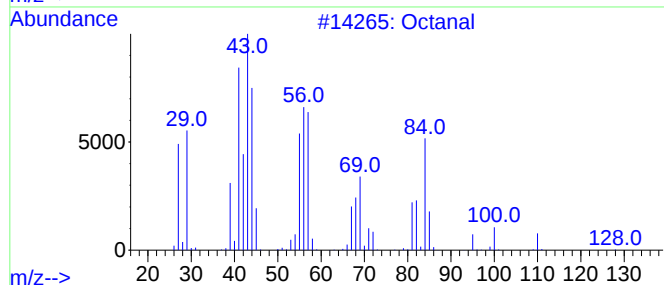
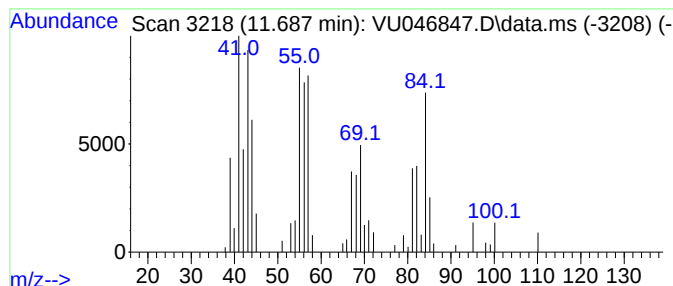
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	1.12 ug/L	76394	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	83
3	Octanal			128	C8H16O	000124-13-0	72
4	Octanal			128	C8H16O	000124-13-0	64
5	1-Pentene, 2-methyl-			84	C6H12	000763-29-1	43



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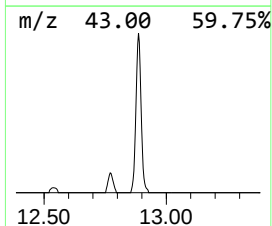
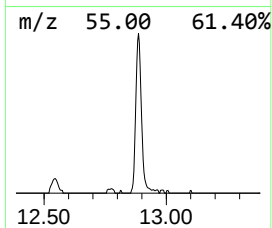
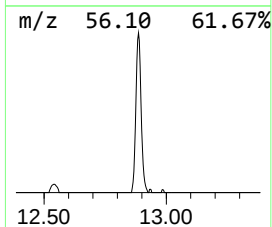
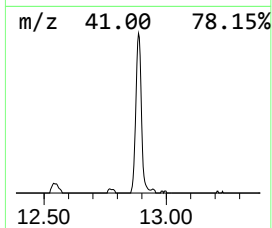
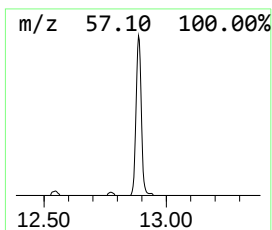
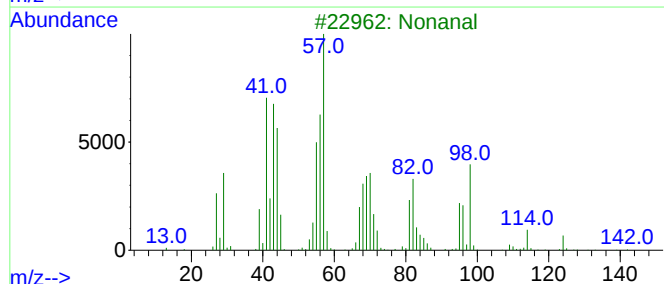
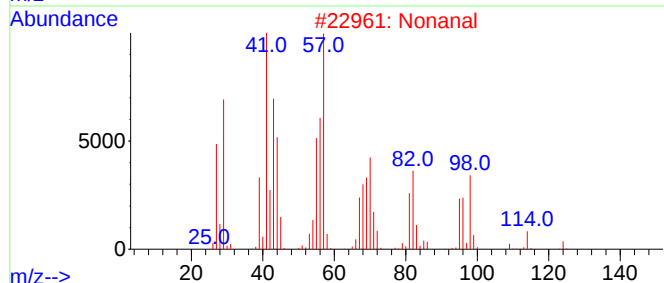
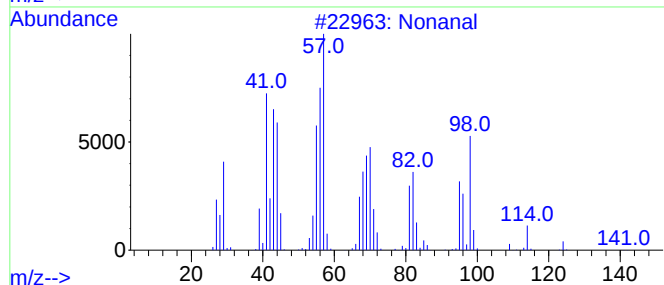
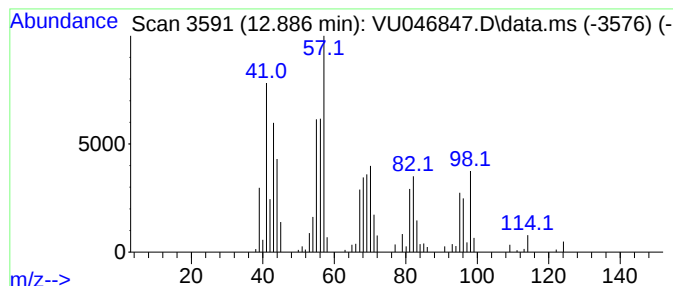
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	2.35 ug/L	160783	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	80
4			2-Nonen-1-ol	142	C9H18O	022104-79-6	35
5			11-Hexadecen-1-ol, (Z)-	240	C16H32O	056683-54-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012622\
Data File : VU046847.D
Acq On : 26 Jan 2022 15:49
Operator : SY/MD
Sample : N1260-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.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
unknown-01	1.475	0.6	ug/L	27551	1	6.253	228275	5.0
Pentanal	6.880	0.9	ug/L	41514	1	6.253	228275	5.0
Hexanal	8.787	4.9	ug/L	305529	2	9.420	314536	5.0
Heptanal	10.343	0.8	ug/L	50252	2	9.420	314536	5.0
Octanal	11.687	1.1	ug/L	76394	3	11.812	341679	5.0
Nonanal	12.886	2.4	ug/L	160783	3	11.812	341679	5.0