

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
 Data File : VU046746.D
 Acq On : 12 Jan 2022 16:43
 Operator : SY/MD
 Sample : N1101-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXW7

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: VU046746.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	72	81	93	rBV	26928	32972	2.16%	0.606%
2	1.919	171	180	199	rVB	21486	29728	1.95%	0.546%
3	2.575	368	384	399	rBV5	60869	122393	8.02%	2.250%
4	4.652	1012	1030	1088	rBV	36978	172039	11.28%	3.162%
5	5.067	1144	1159	1182	rVB	47262	108773	7.13%	1.999%
6	5.321	1222	1238	1253	rBB2	25702	57828	3.79%	1.063%
7	5.729	1343	1365	1388	rBV2	88654	235978	15.47%	4.337%
8	6.250	1514	1527	1545	rBV	91829	171660	11.25%	3.155%
9	6.694	1652	1665	1683	rBV2	57610	113081	7.41%	2.078%
10	6.883	1713	1724	1745	rBV2	17161	36067	2.36%	0.663%
11	7.568	1925	1937	1949	rBV	29262	51079	3.35%	0.939%
12	7.899	2026	2040	2054	rBV	103539	180086	11.80%	3.310%
13	8.182	2117	2128	2143	rBV2	18624	30815	2.02%	0.566%
14	8.555	2229	2244	2258	rBV	199728	338130	22.16%	6.215%
15	8.636	2258	2269	2304	rVV	207319	379368	24.86%	6.973%
16	8.787	2304	2316	2348	rVV	154369	268680	17.61%	4.938%
17	9.417	2499	2512	2532	rBV	138481	228408	14.97%	4.198%
18	10.343	2789	2800	2820	rBV	72649	117724	7.72%	2.164%
19	10.758	2918	2929	2943	rBV	63660	100076	6.56%	1.839%
20	11.687	3206	3218	3245	rBV	376844	559331	36.66%	10.280%
21	11.812	3245	3257	3274	rVB	175089	277640	18.20%	5.103%
22	12.192	3364	3375	3389	rBV	125860	203174	13.32%	3.734%
23	12.542	3473	3484	3502	rBV3	24674	48532	3.18%	0.892%
24	12.886	3579	3591	3616	rBV	1056028	1525755	100.00%	28.043%
25	14.732	4156	4165	4179	rVB2	35290	51473	3.37%	0.946%

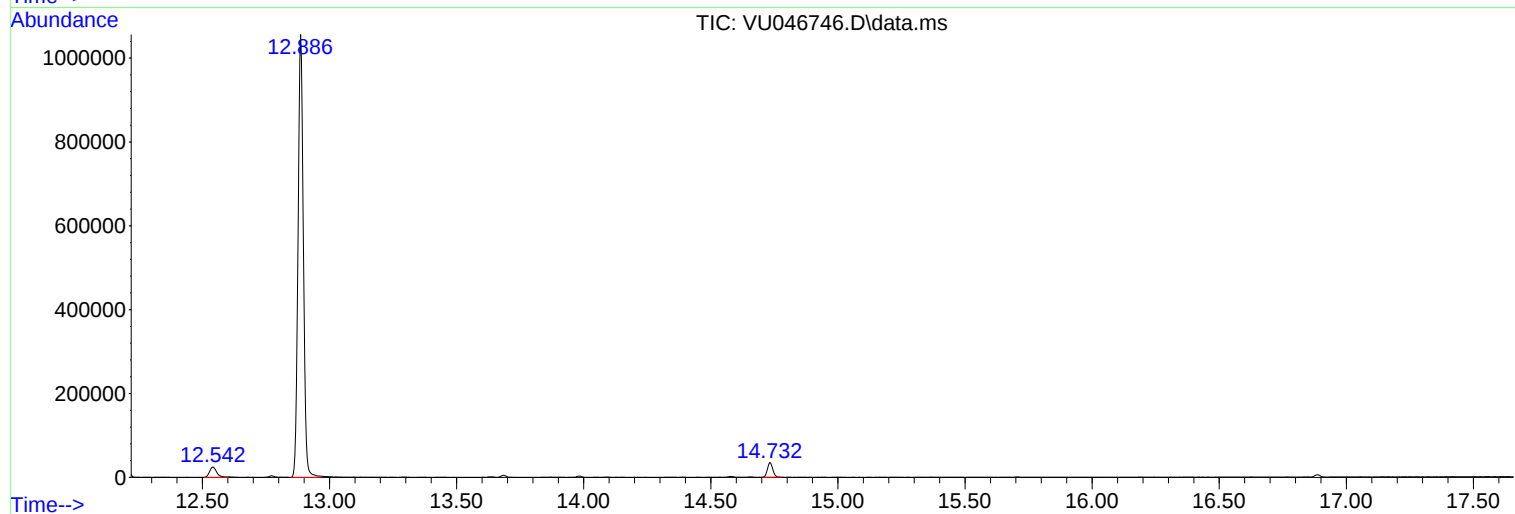
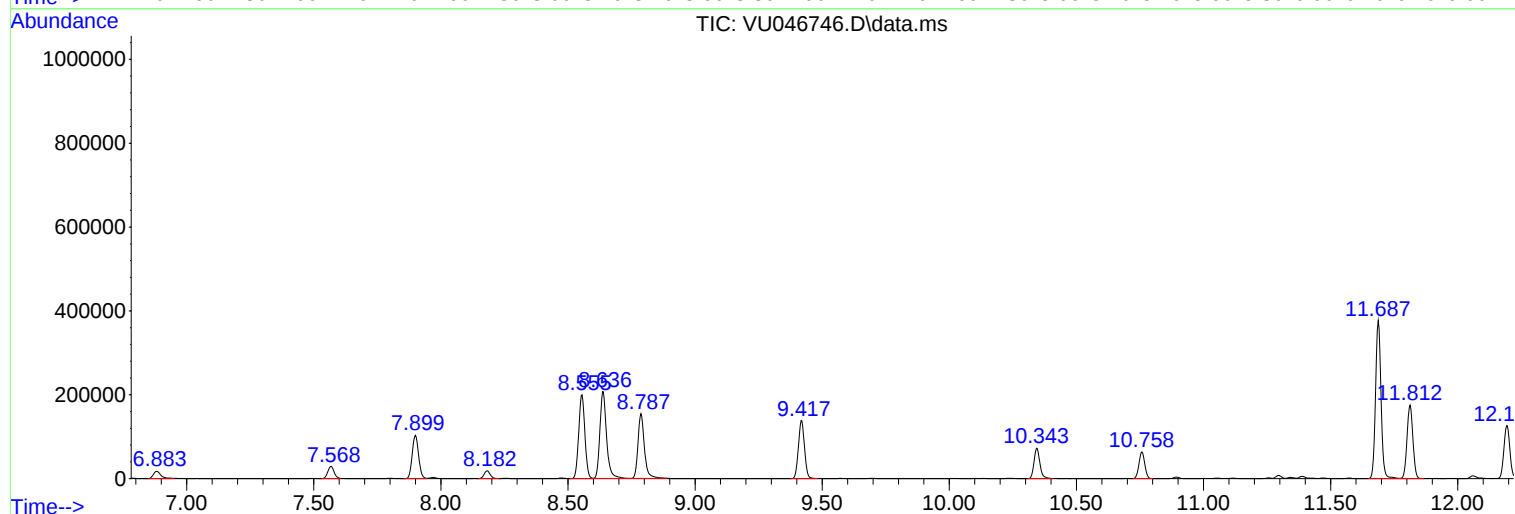
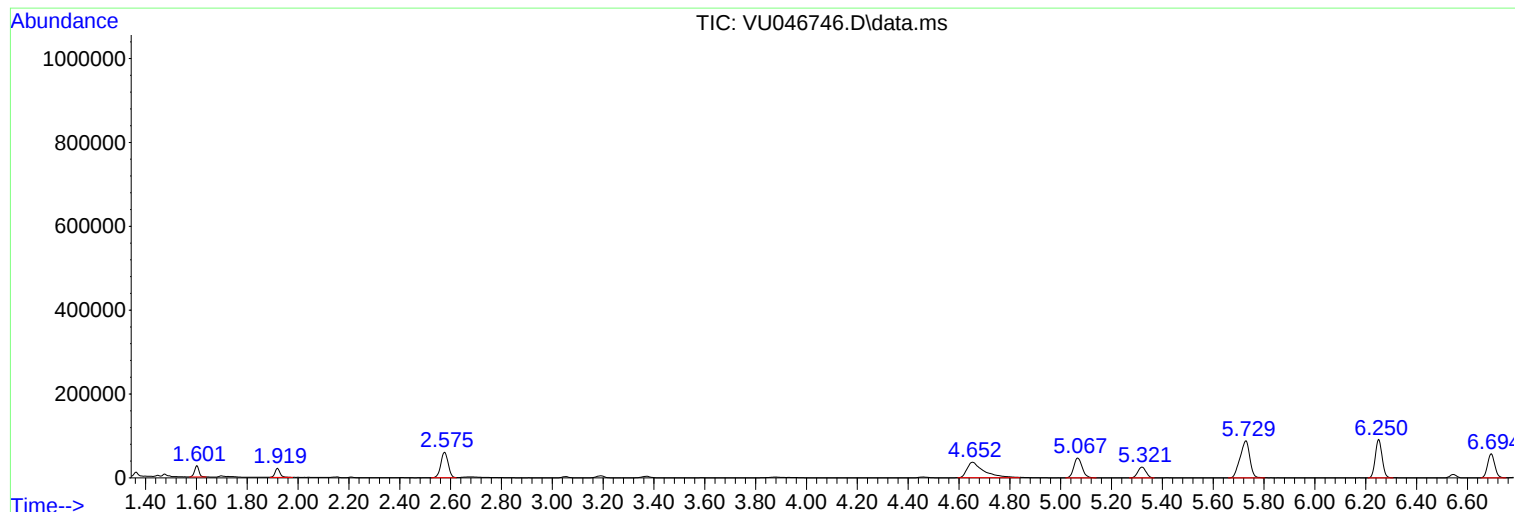
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW7

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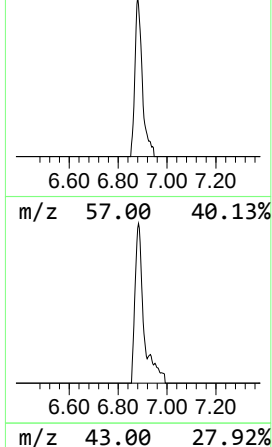
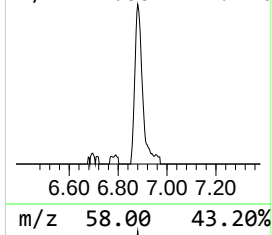
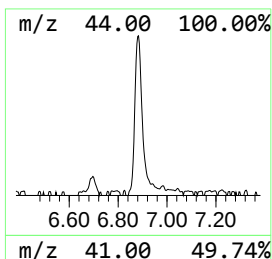
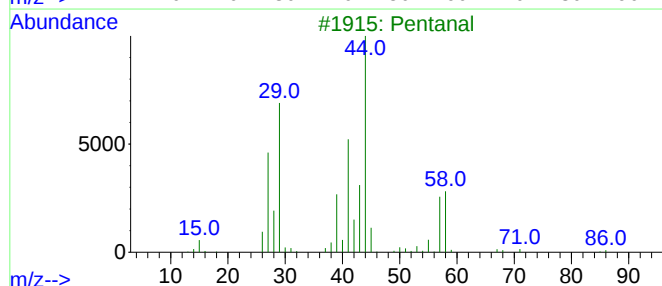
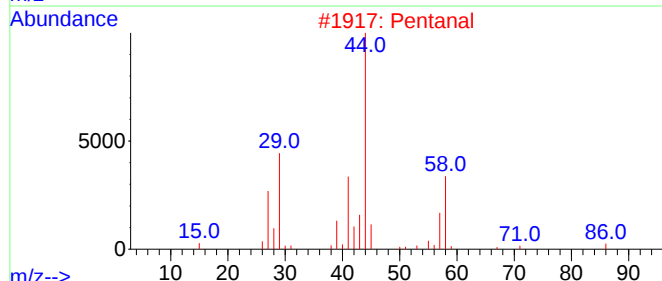
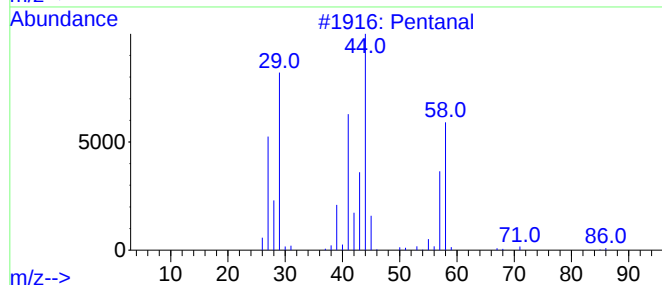
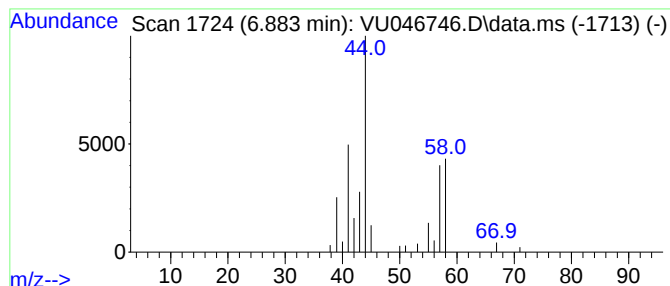
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	1.05 ug/L	36067	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	56
2	Pentanal			86	C5H10O	000110-62-3	40
3	Pentanal			86	C5H10O	000110-62-3	9
4	1-Octadecanamine, N-methyl-			283	C19H41N	002439-55-6	9
5	Ethylene oxide			44	C2H4O	000075-21-8	5



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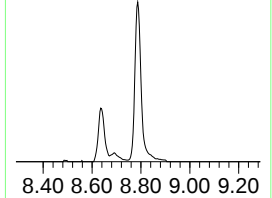
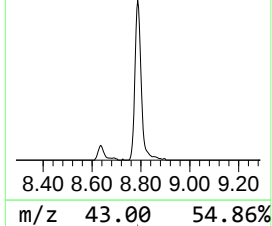
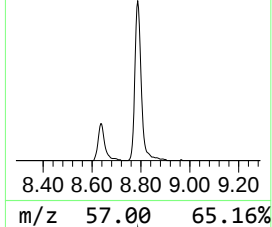
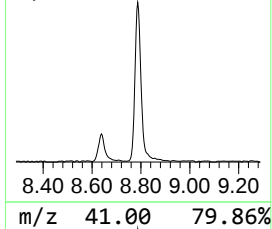
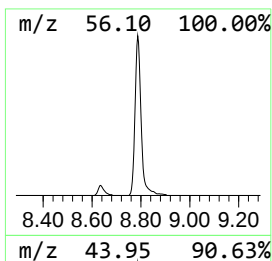
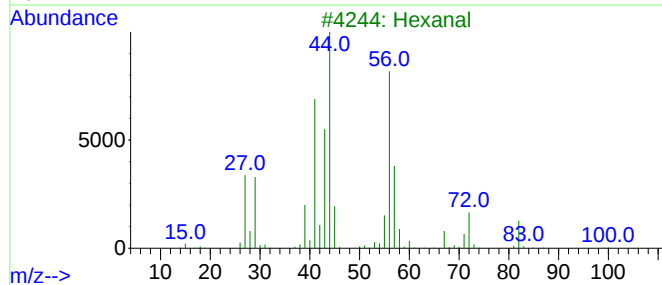
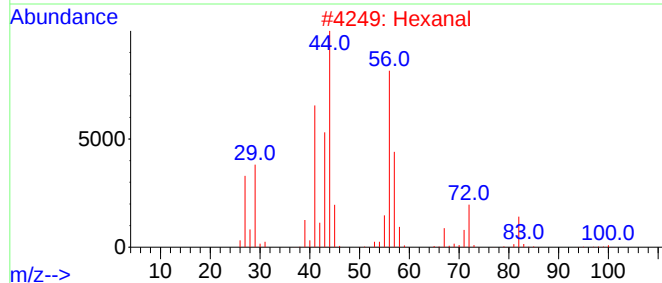
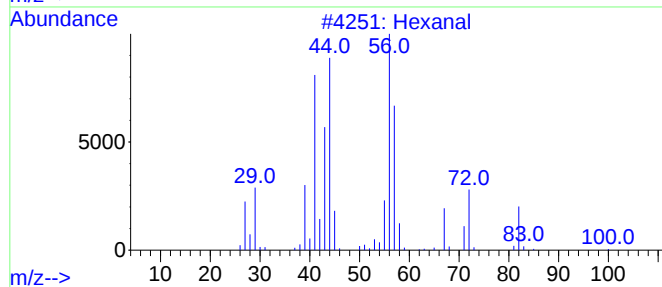
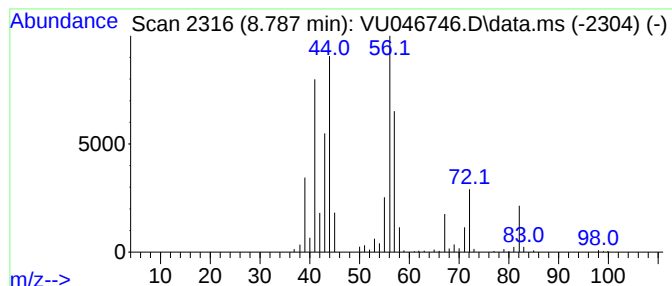
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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	5.88 ug/L	268680	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	91
4	Hexanal			100	C6H12O	000066-25-1	83
5	Hexanal			100	C6H12O	000066-25-1	72



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW7

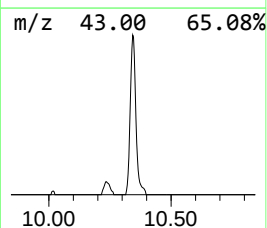
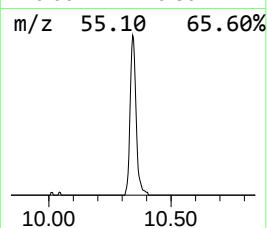
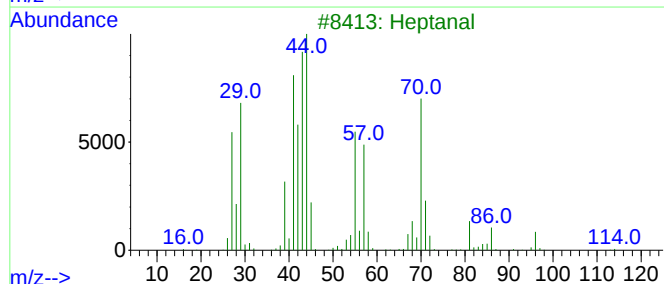
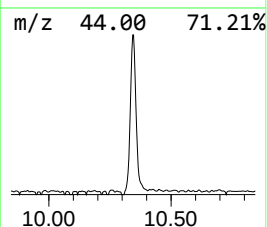
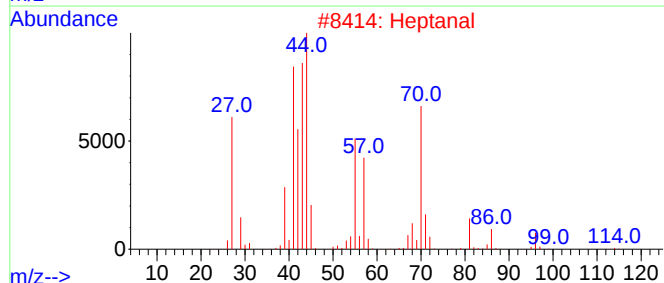
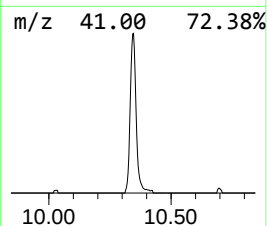
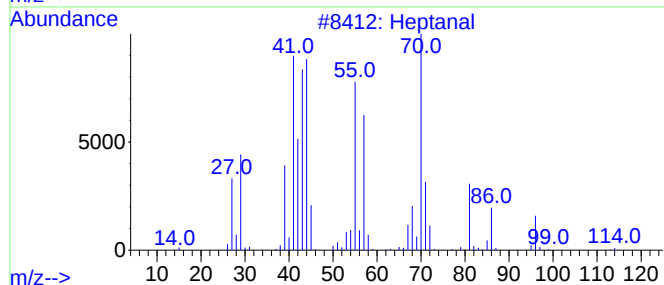
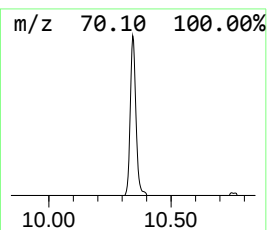
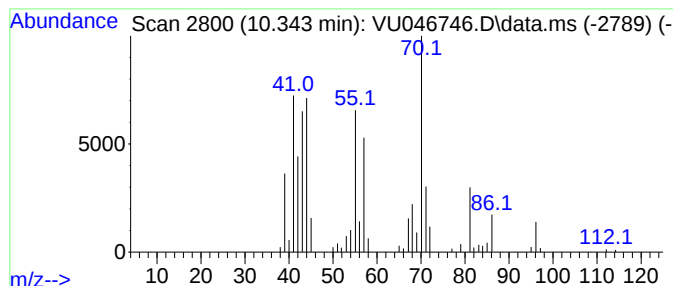
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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	2.58 ug/L	117724	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	97
2	Heptanal			114	C7H14O	000111-71-7	95
3	Heptanal			114	C7H14O	000111-71-7	95
4	Heptanal			114	C7H14O	000111-71-7	64
5	Heptanal			114	C7H14O	000111-71-7	52



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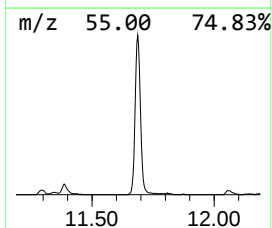
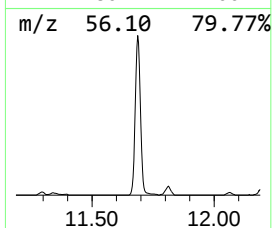
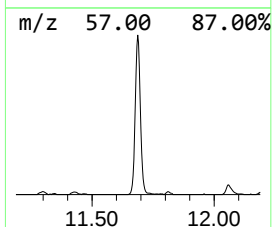
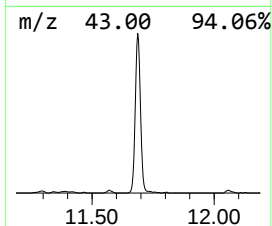
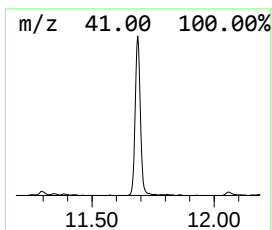
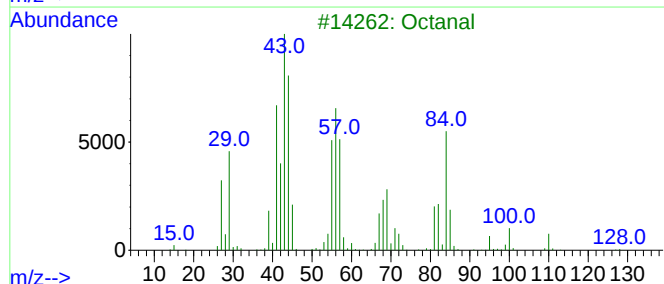
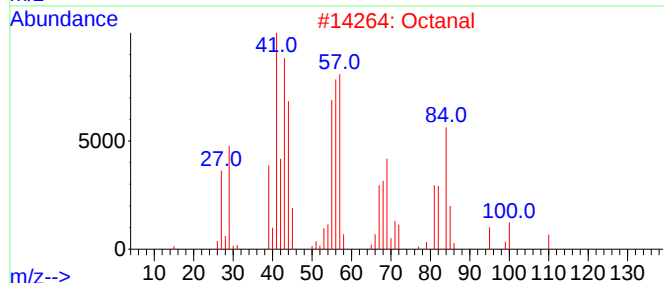
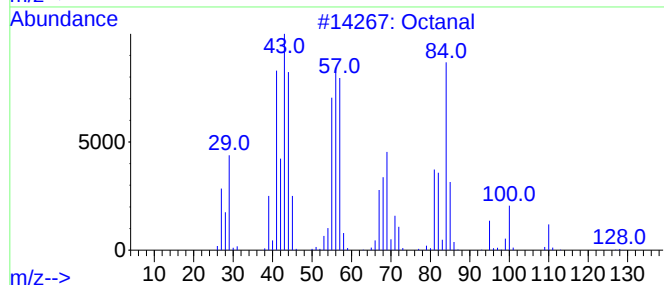
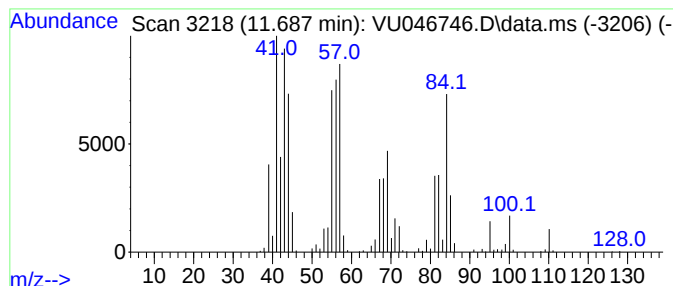
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	10.07 ug/L	559331	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	50
5	Cyclopentanol, 2-methyl-, cis-			100	C6H12O	025144-05-2	42



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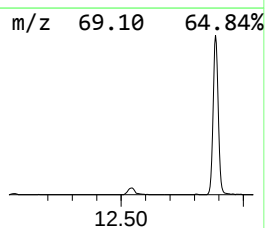
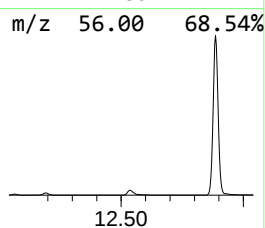
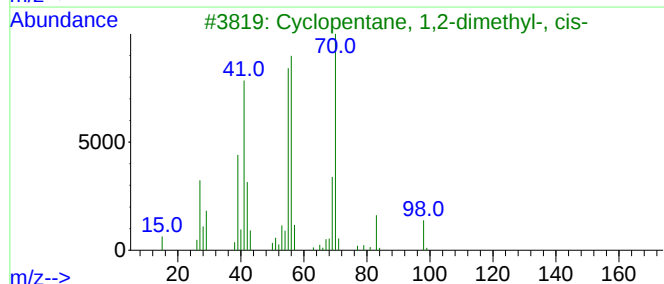
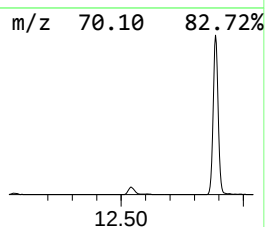
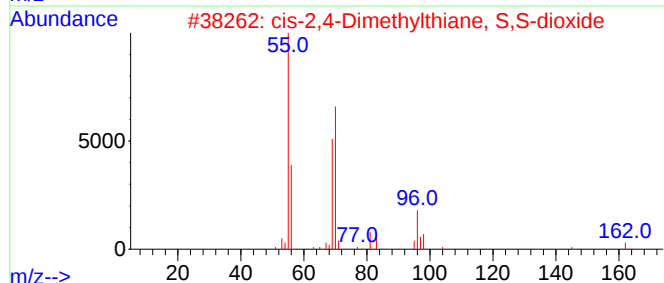
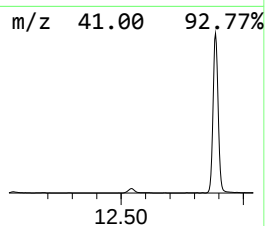
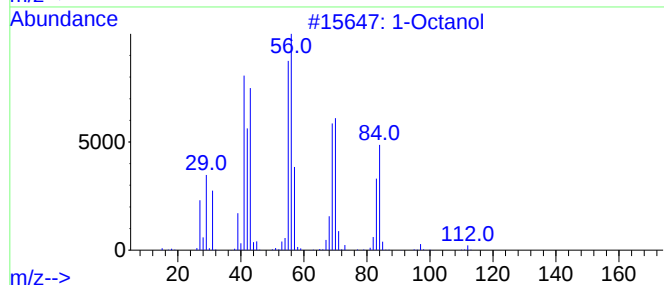
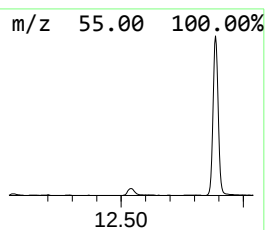
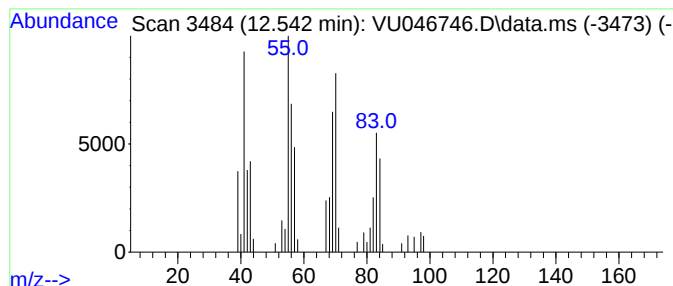
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.542	0.87 ug/L	48532	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	43
2			cis-2,4-Dimethylthiane, S,S-dioxide	162	C7H14O2S	1000215-67-5	43
3			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	43
4			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	43
5			2-Hexenal, (E)-	98	C6H10O	006728-26-3	38



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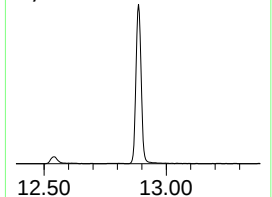
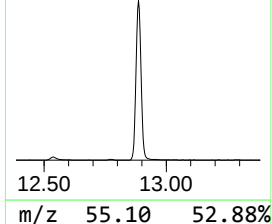
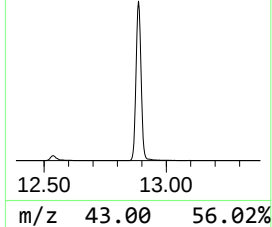
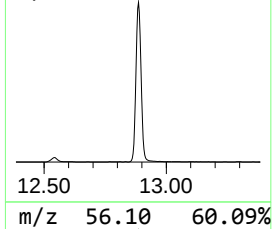
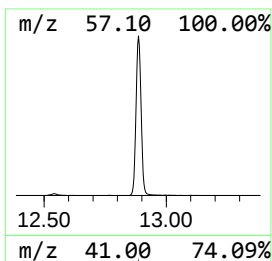
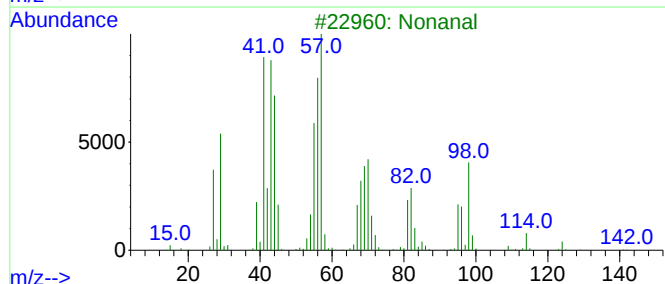
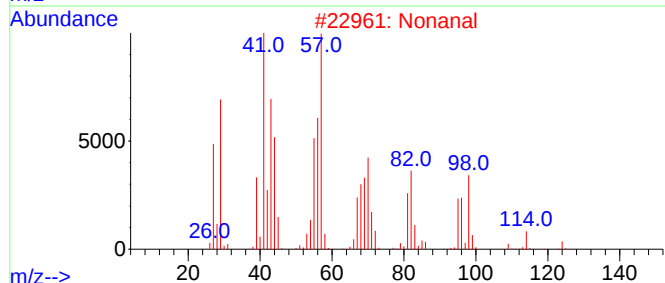
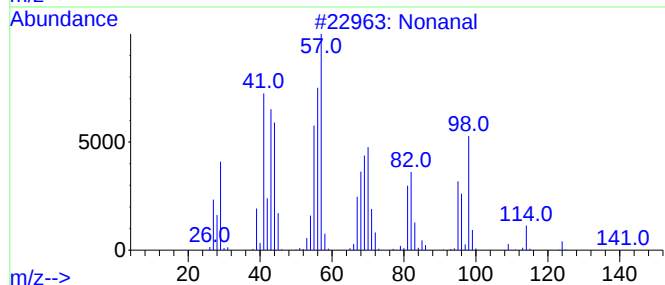
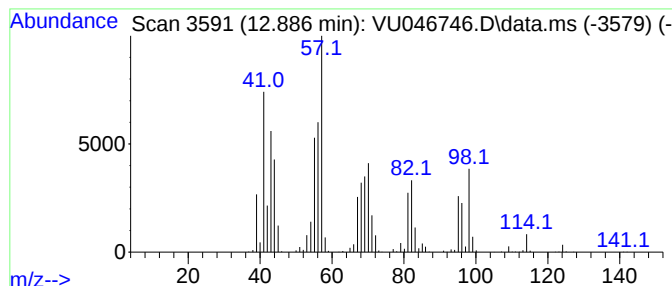
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Quant Title : TRACE VOA SFAM1.0

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	27.48 ug/L	1525760	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	87
3			Nonanal	142	C9H18O	000124-19-6	83
4			Nonanal	142	C9H18O	000124-19-6	80
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046746.D
Acq On : 12 Jan 2022 16:43
Operator : SY/MD
Sample : N1101-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW7

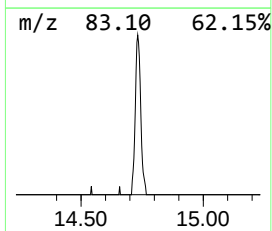
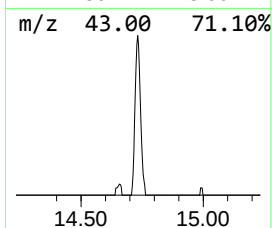
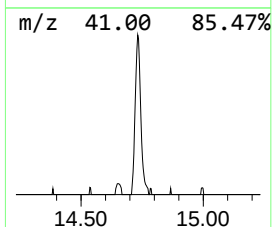
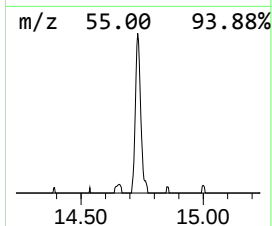
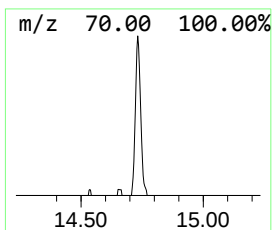
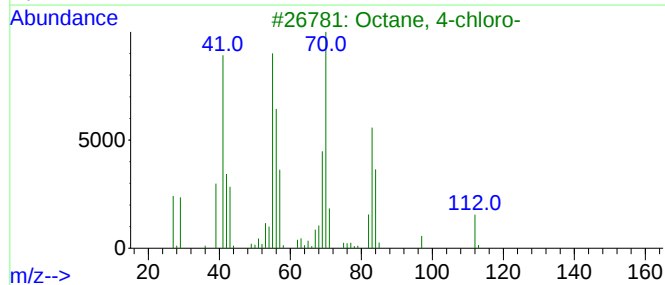
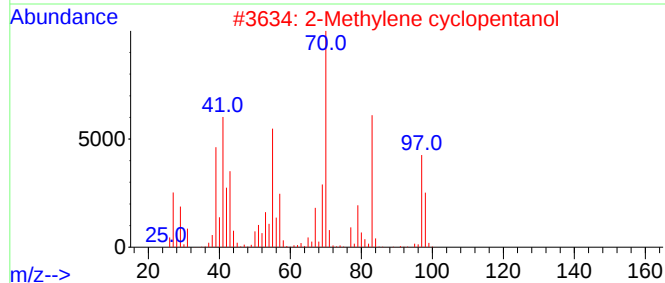
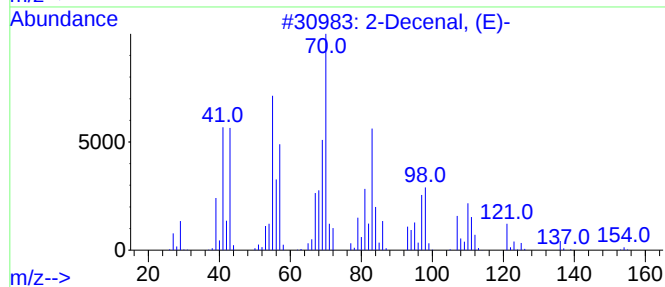
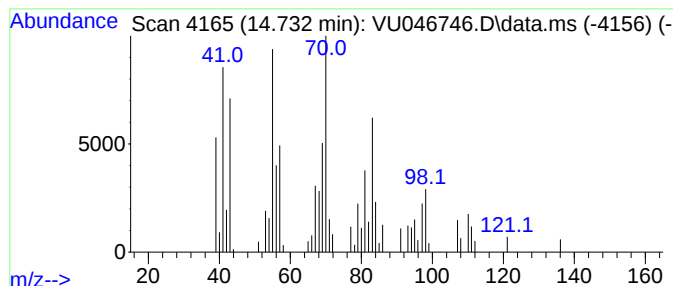
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 2-Decenal, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.732	0.93 ug/L	51473	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decenal, (E)-	154	C10H18O	003913-81-3	80
2			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	49
3			Octane, 4-chloro-	148	C8H17Cl	000999-07-5	47
4			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	46
5			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046746.D
Acq On : 12 Jan 2022 16:43
Operator : SY/MD
Sample : N1101-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW7

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	6.883	1.1	ug/L	36067	1	6.250	171660	5.0
Hexanal	8.787	5.9	ug/L	268680	2	9.417	228408	5.0
Heptanal	10.343	2.6	ug/L	117724	2	9.417	228408	5.0
Octanal	11.687	10.1	ug/L	559331	3	11.812	277640	5.0
unknown-01	12.542	0.9	ug/L	48532	3	11.812	277640	5.0
Nonanal	12.886	27.5	ug/L	1525760	3	11.812	277640	5.0
2-Decenal, (E)-	14.732	0.9	ug/L	51473	3	11.812	277640	5.0