

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
 Data File : VU046742.D
 Acq On : 12 Jan 2022 15:07
 Operator : SY/MD
 Sample : N1077-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXW3

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: VU046742.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	71	80	95	rVB	33549	41427	1.38%	0.520%
2	1.925	174	182	198	rVB	21349	30112	1.00%	0.378%
3	2.211	261	271	284	rVB	78470	109014	3.62%	1.368%
4	2.575	364	384	415	rBV3	74082	203369	6.76%	2.552%
5	4.755	1032	1062	1063	rBV3	18749	49541	1.65%	0.622%
6	5.102	1155	1170	1196	rVB2	47858	120465	4.00%	1.512%
7	5.751	1352	1372	1399	rBV2	97806	236437	7.86%	2.967%
8	6.272	1520	1534	1551	rBV	97478	181357	6.03%	2.276%
9	6.713	1659	1671	1685	rBV	57712	112381	3.73%	1.410%
10	6.906	1717	1731	1762	rBV	98390	222599	7.40%	2.794%
11	7.581	1930	1941	1964	rVB	30798	51185	1.70%	0.642%
12	7.909	2027	2043	2058	rBV	107139	185041	6.15%	2.322%
13	8.652	2255	2274	2305	rBV	170243	350077	11.63%	4.394%
14	8.796	2305	2319	2367	rVB	1644899	3009353	100.00%	37.769%
15	9.423	2502	2514	2529	rBV	139842	232530	7.73%	2.918%
16	10.349	2792	2802	2825	rVB	103419	175087	5.82%	2.197%
17	10.761	2919	2930	2944	rVB	59678	96473	3.21%	1.211%
18	11.298	3088	3097	3109	rVB2	68960	107401	3.57%	1.348%
19	11.690	3206	3219	3236	rBV	256989	387228	12.87%	4.860%
20	11.812	3246	3257	3273	rVB	180502	287277	9.55%	3.605%
21	12.063	3324	3335	3353	rBV2	23428	45222	1.50%	0.568%
22	12.195	3364	3376	3387	rBV	127324	201321	6.69%	2.527%
23	12.545	3472	3485	3514	rBV	202509	328617	10.92%	4.124%
24	12.886	3574	3591	3607	rBV	225552	331337	11.01%	4.158%
25	13.684	3830	3839	3855	rVB2	42640	65717	2.18%	0.825%
26	14.732	4152	4165	4184	rBV	427390	619903	20.60%	7.780%
27	15.709	4457	4469	4483	rBV2	97357	149272	4.96%	1.873%
28	16.876	4819	4832	4843	rBV6	20676	38037	1.26%	0.477%

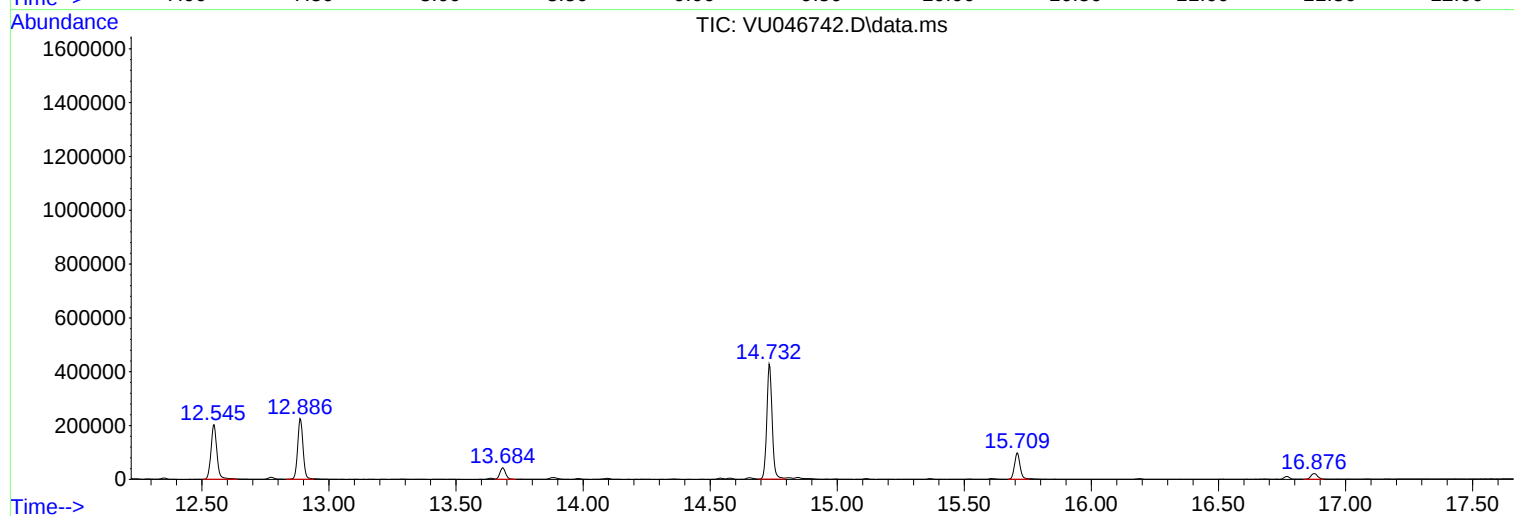
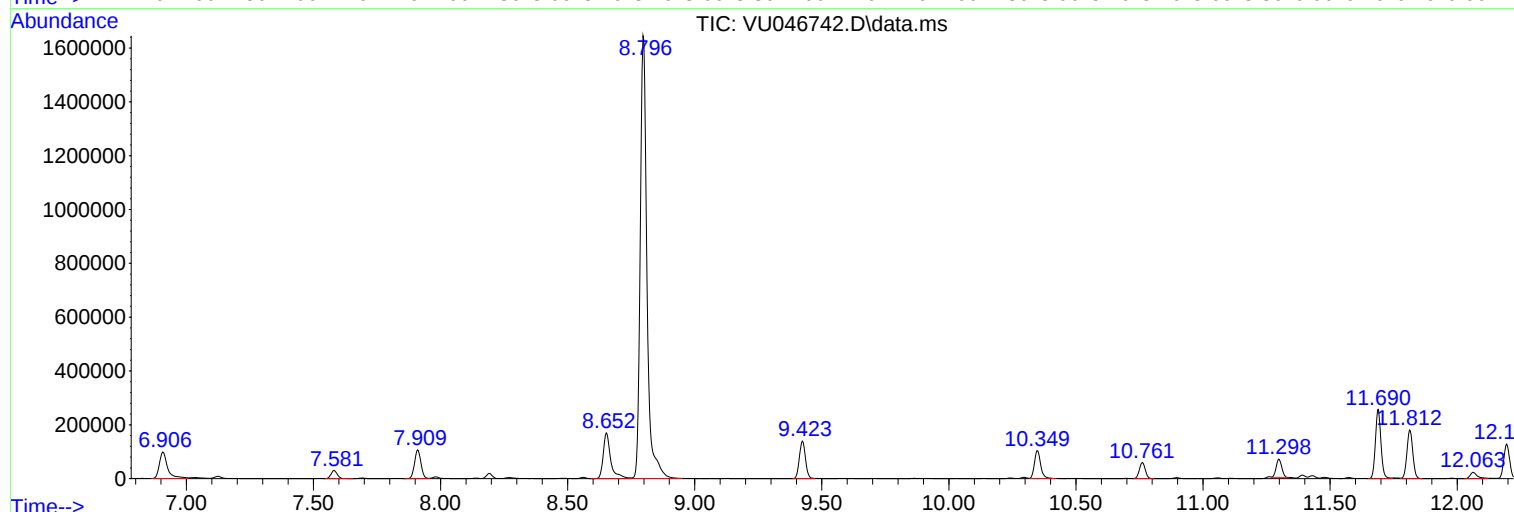
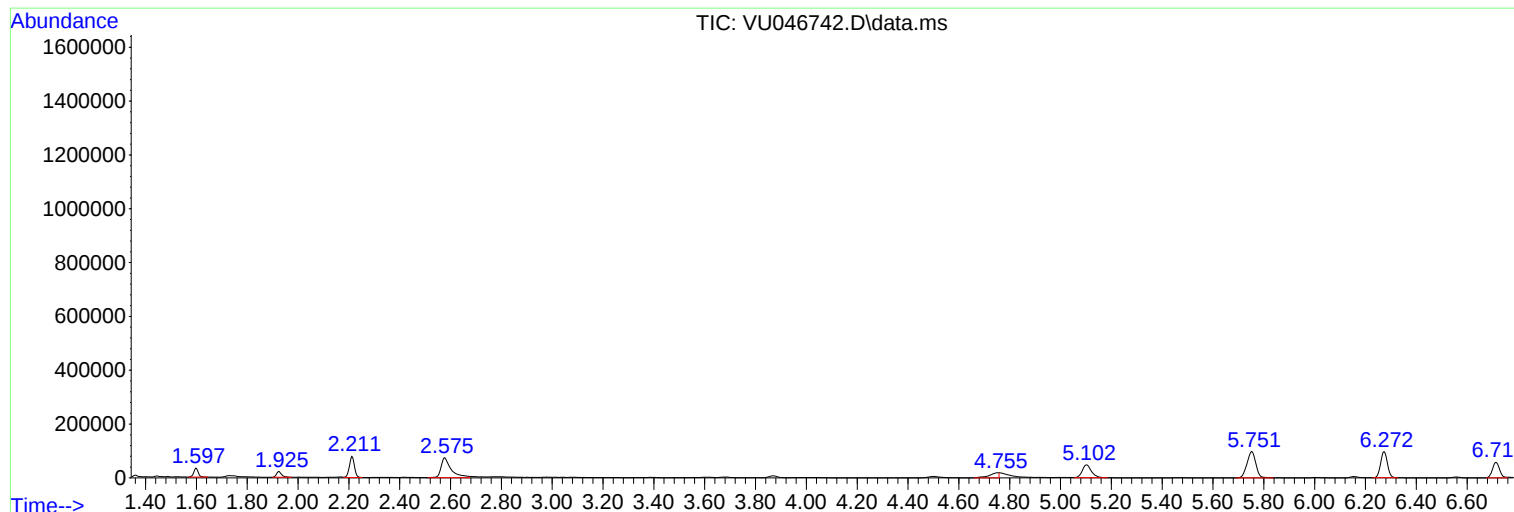
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Instrument :
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ClientSampleId :
BFXW3

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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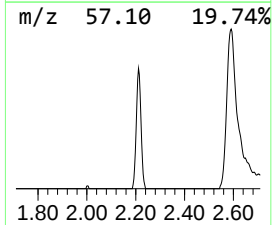
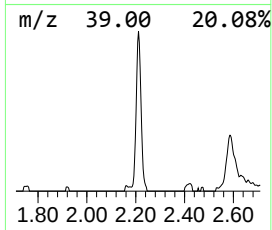
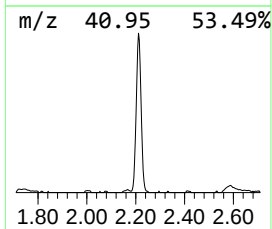
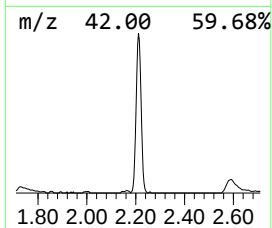
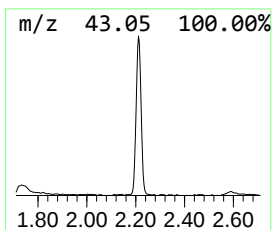
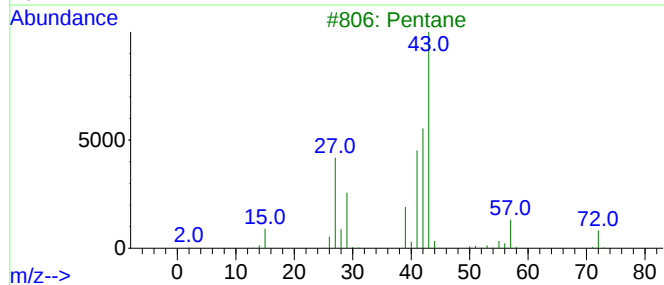
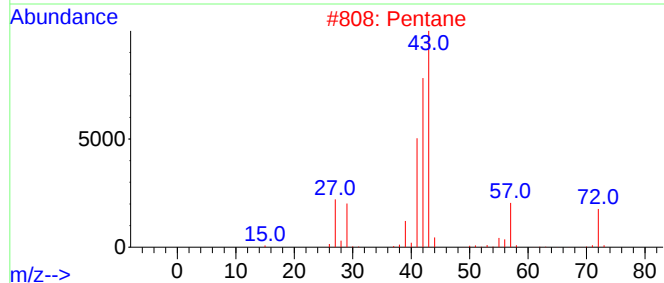
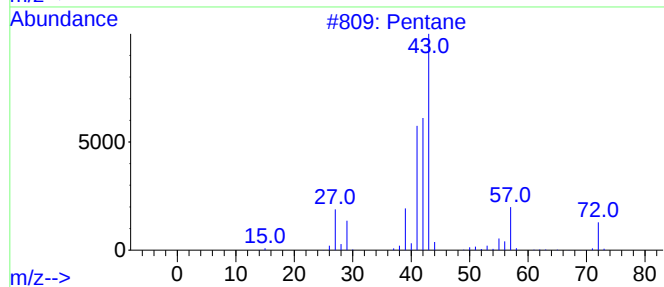
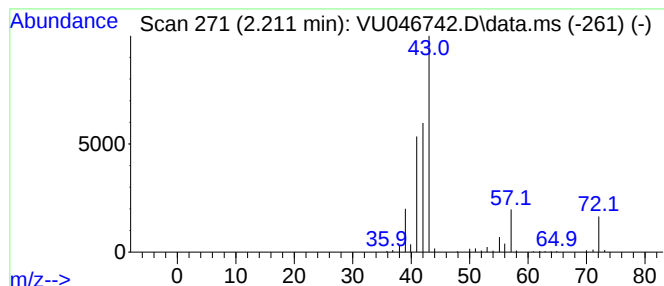
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	3.01 ug/L	109014	1,4-Difluorobenzene	6.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	91
2	Pentane			72	C5H12	000109-66-0	90
3	Pentane			72	C5H12	000109-66-0	86
4	Pentane			72	C5H12	000109-66-0	86
5	Pentane			72	C5H12	000109-66-0	64



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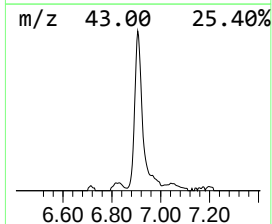
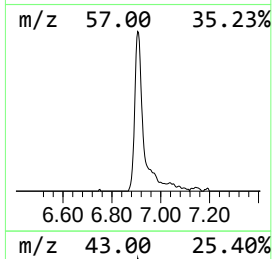
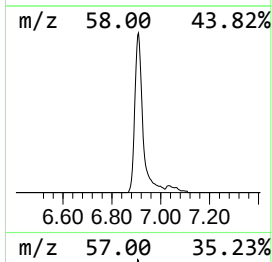
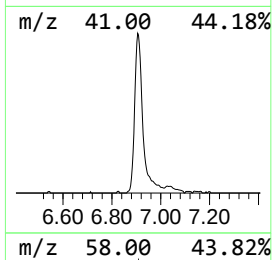
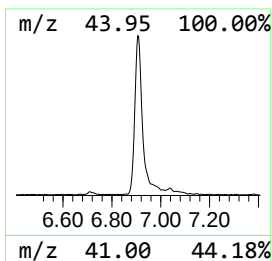
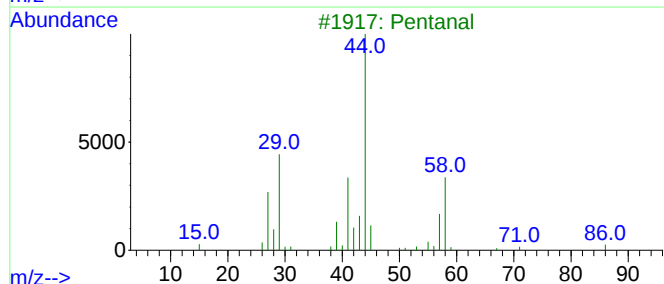
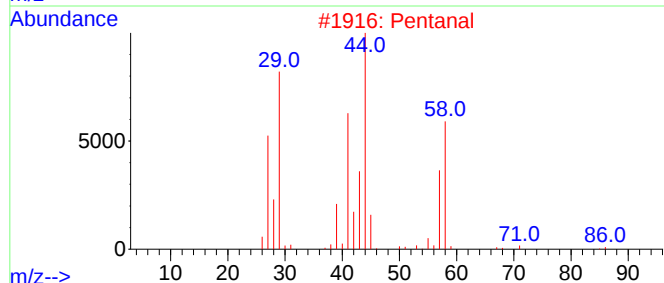
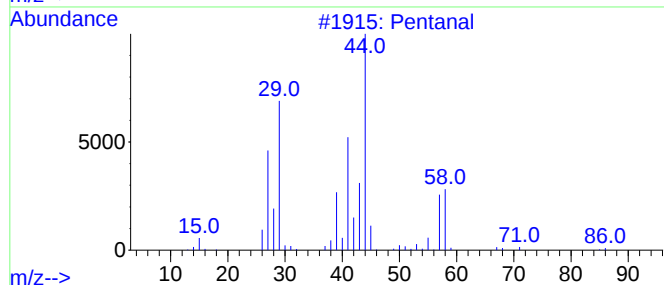
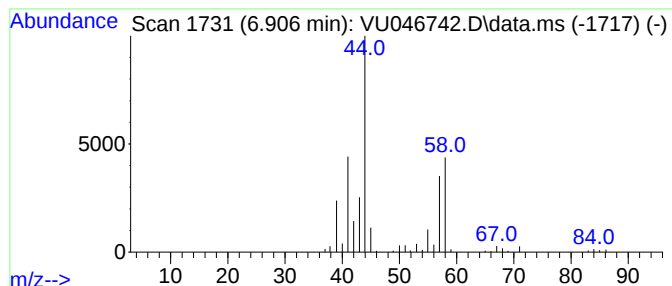
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.906	6.14 ug/L	222599	1,4-Difluorobenzene	6.272

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	86
2	Pentanal			86	C5H10O	000110-62-3	86
3	Pentanal			86	C5H10O	000110-62-3	83
4	Butanal, 3-methyl-			86	C5H10O	000590-86-3	74
5	Pentanal			86	C5H10O	000110-62-3	64



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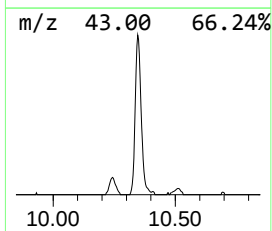
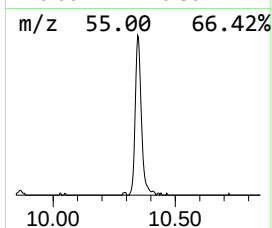
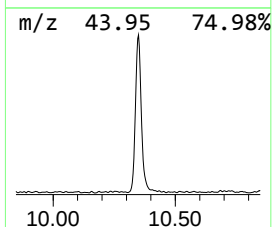
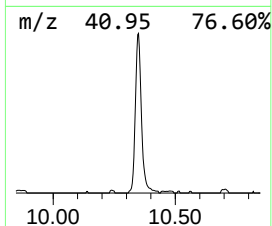
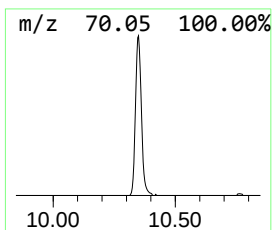
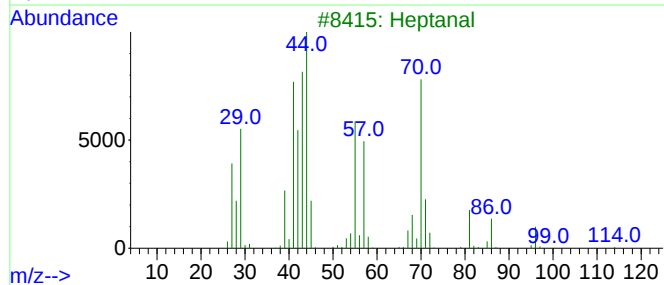
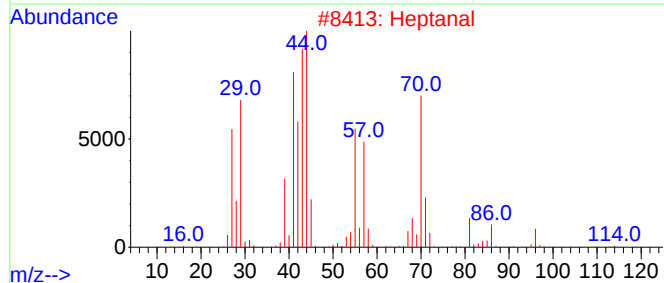
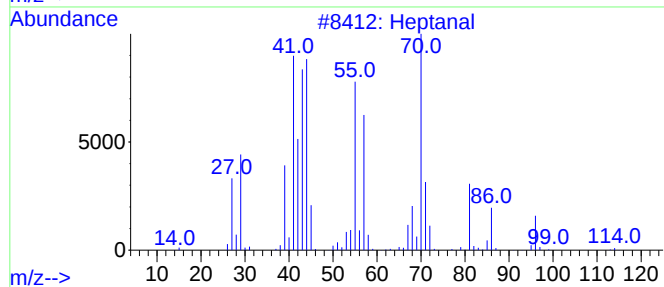
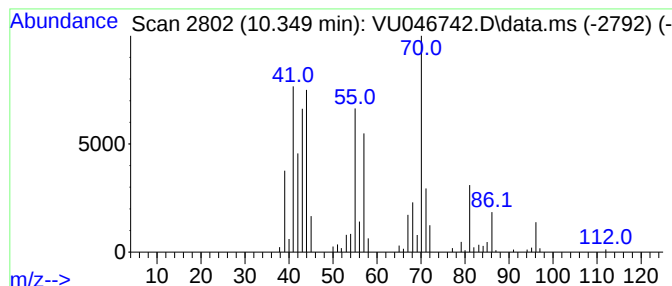
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.349	3.76 ug/L	175087	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	91
2	Heptanal			114	C7H14O	000111-71-7	83
3	Heptanal			114	C7H14O	000111-71-7	83
4	Heptanal			114	C7H14O	000111-71-7	83
5	Heptanal			114	C7H14O	000111-71-7	78



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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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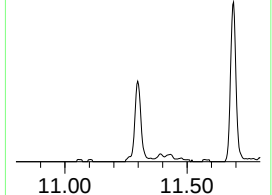
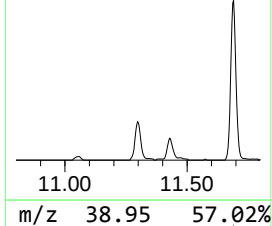
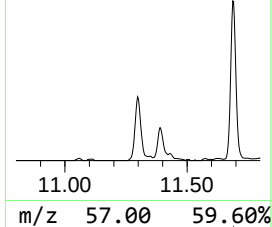
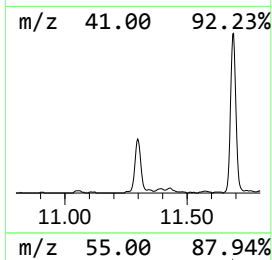
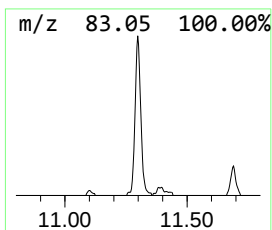
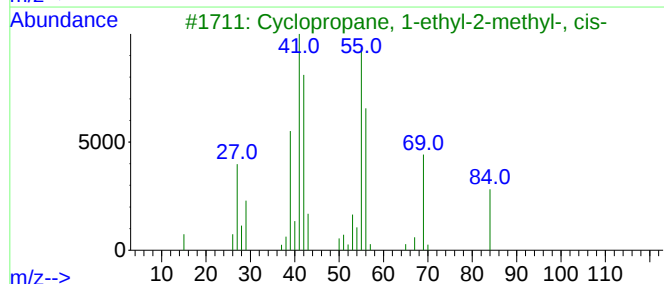
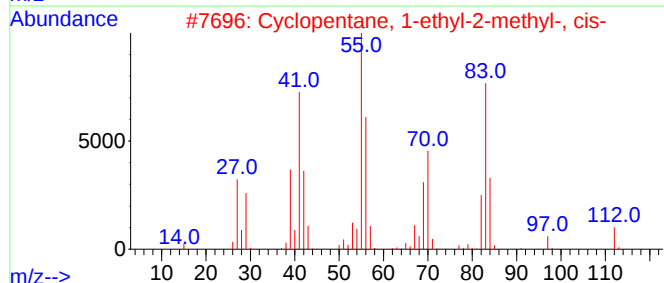
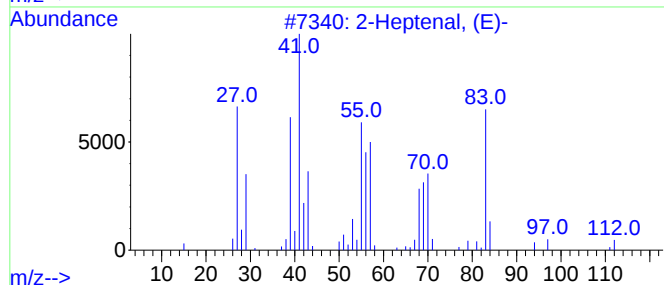
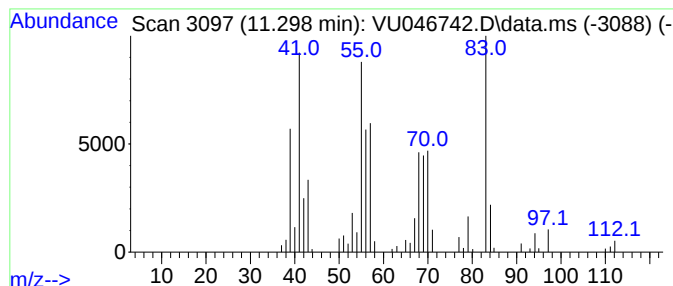
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Heptenal, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	1.87 ug/L	107401	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptenal, (E)-	112	C7H12O	018829-55-5	91
2			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	58
3			Cyclopropane, 1-ethyl-2-methyl-,...	84	C6H12	019781-68-1	51
4			2-Heptenal, (Z)-	112	C7H12O	057266-86-1	47
5			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	47



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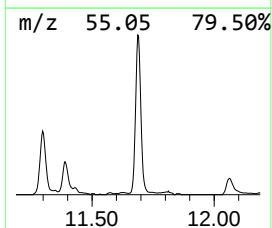
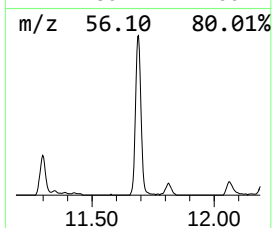
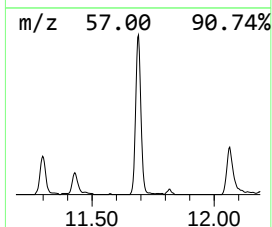
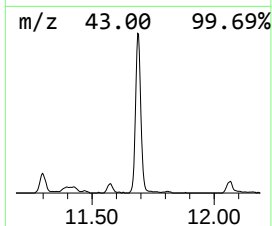
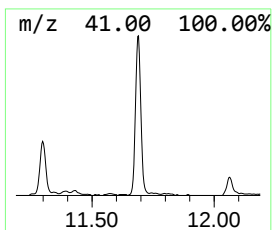
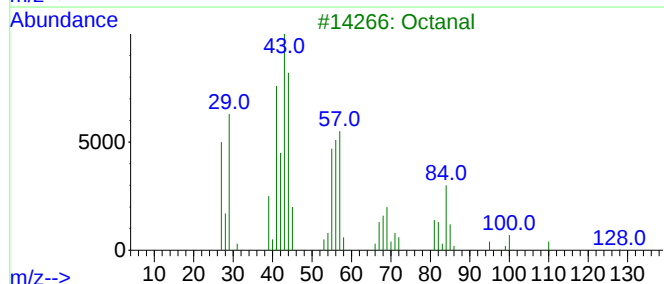
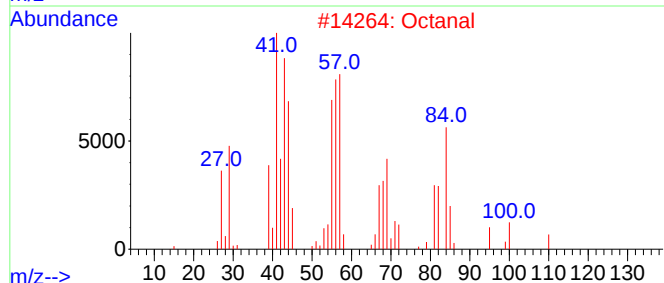
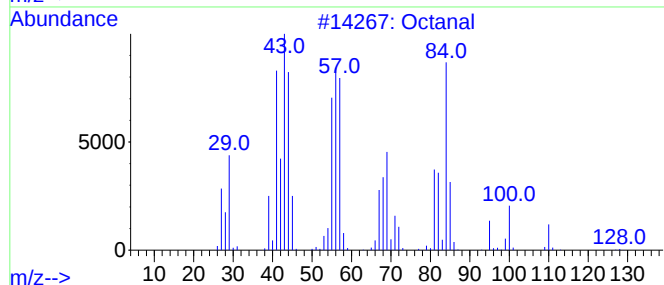
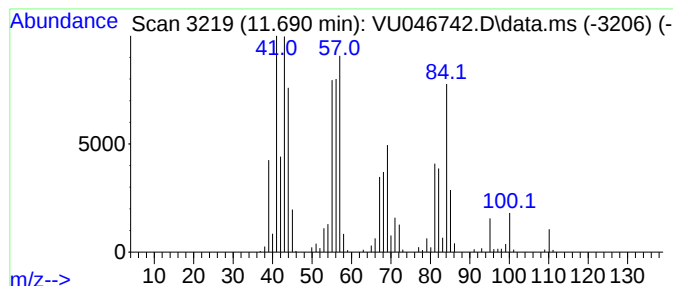
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.690	6.74 ug/L	387228	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	91
2	Octanal			128	C8H16O	000124-13-0	91
3	Octanal			128	C8H16O	000124-13-0	83
4	Octanal			128	C8H16O	000124-13-0	83
5	Cyclopentanol, 2-methyl-, cis-			100	C6H12O	025144-05-2	46



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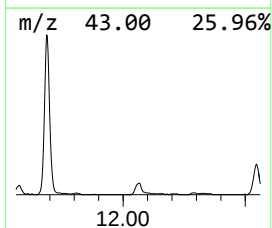
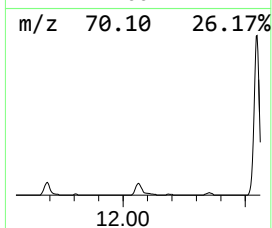
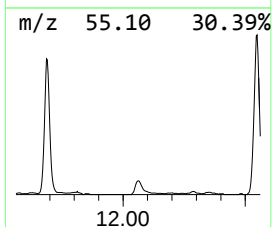
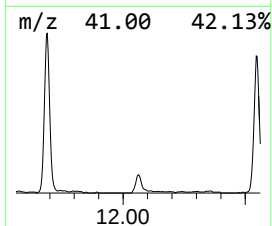
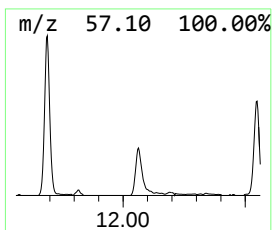
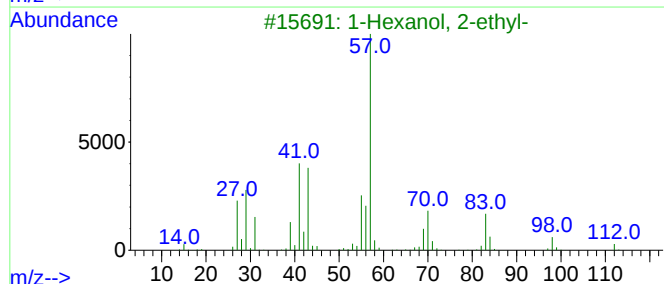
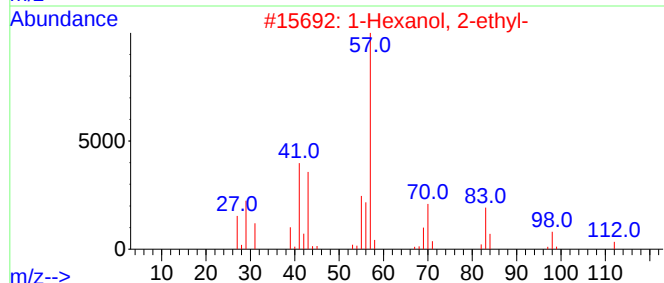
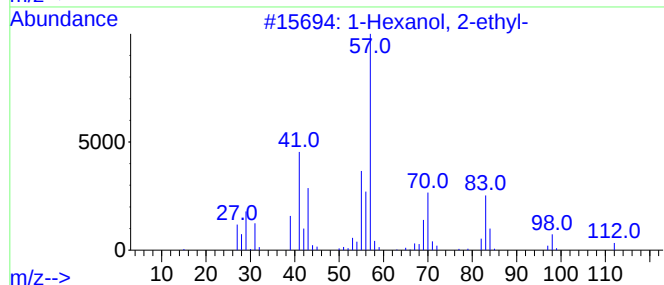
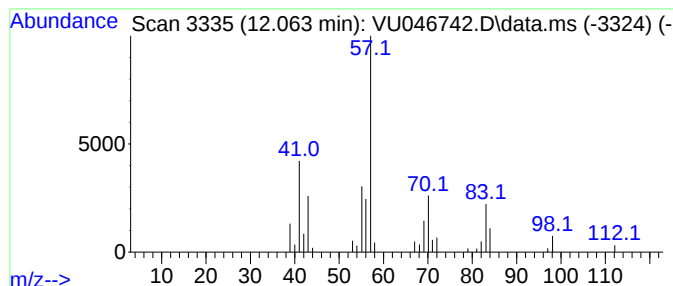
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	0.79 ug/L	45222	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046742.D
Acq On : 12 Jan 2022 15:07
Operator : SY/MD
Sample : N1077-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW3

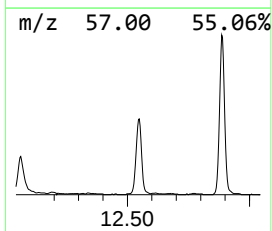
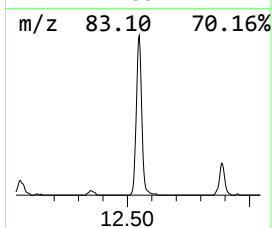
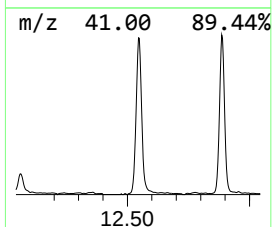
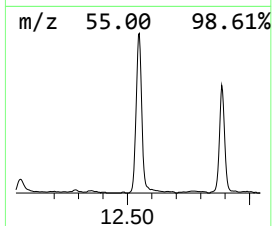
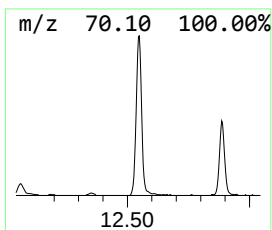
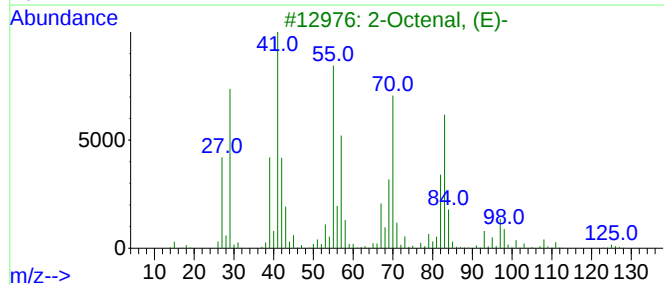
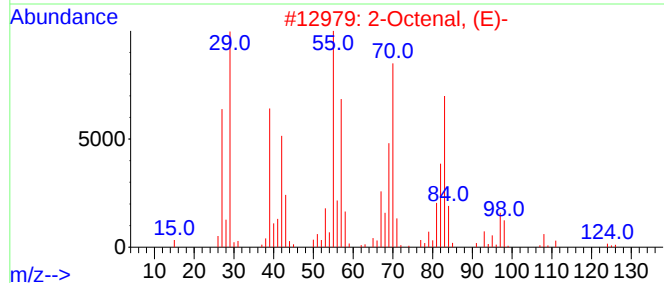
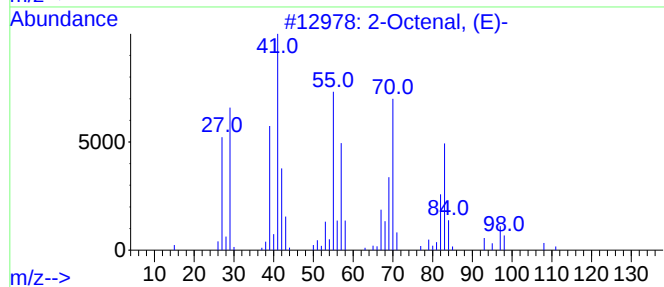
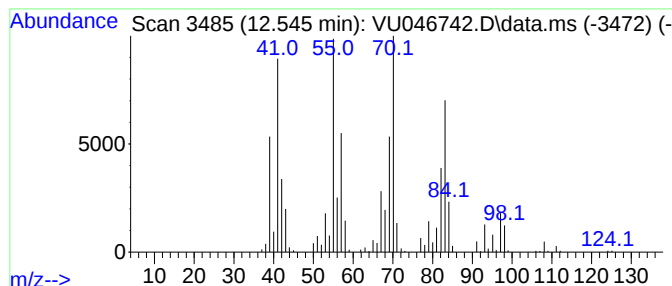
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 2-Octenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	5.72 ug/L	328617	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octenal, (E)-	126	C8H14O	002548-87-0	86
2			2-Octenal, (E)-	126	C8H14O	002548-87-0	78
3			2-Octenal, (E)-	126	C8H14O	002548-87-0	78
4			2-Octenal, (E)-	126	C8H14O	002548-87-0	72
5			2-Tridecenal, (E)-	196	C13H24O	007069-41-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046742.D
Acq On : 12 Jan 2022 15:07
Operator : SY/MD
Sample : N1077-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW3

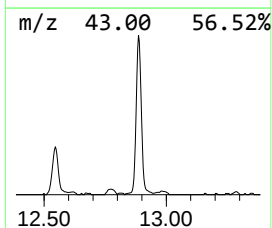
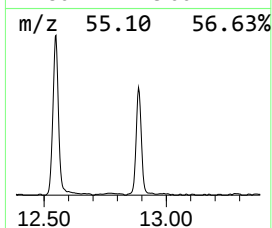
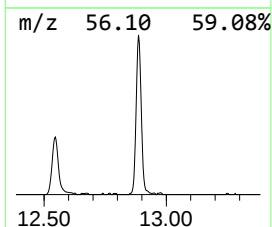
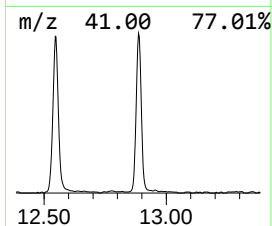
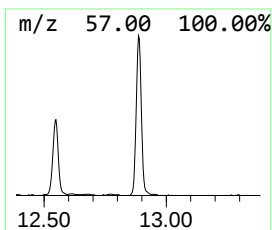
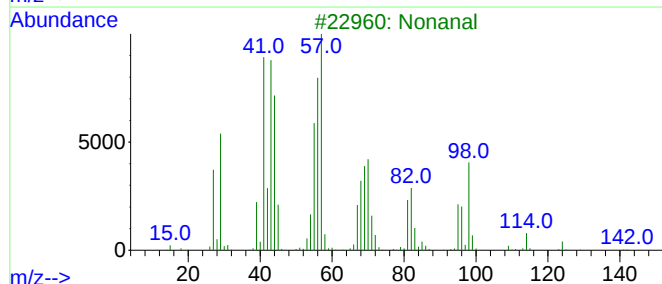
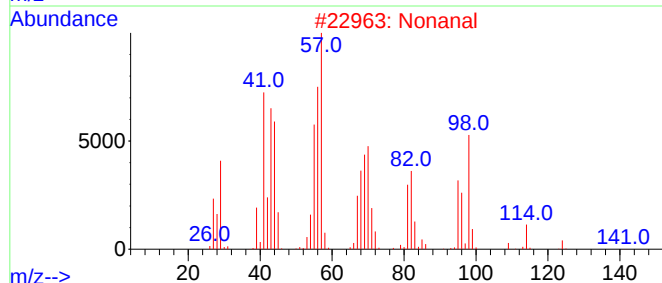
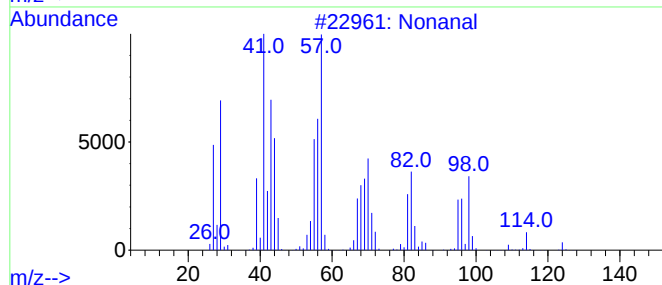
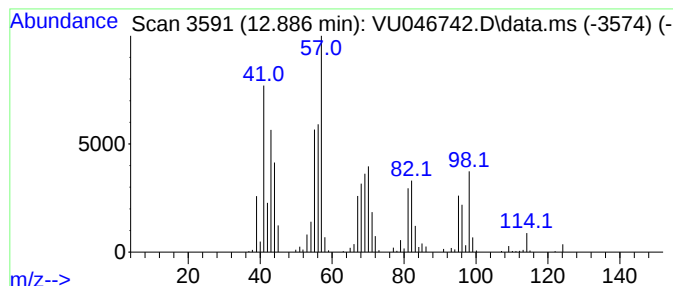
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	5.77 ug/L	331337	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	83
4			Nonanal	142	C9H18O	000124-19-6	72
5			Cyclohexane, methyl-	98	C7H14	000108-87-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046742.D
Acq On : 12 Jan 2022 15:07
Operator : SY/MD
Sample : N1077-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

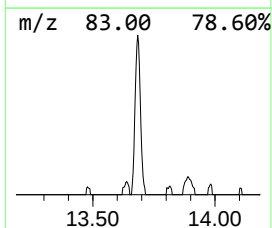
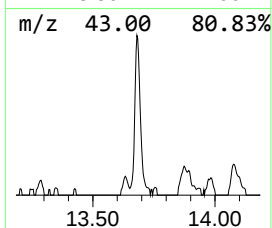
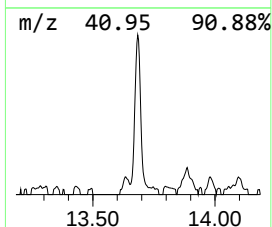
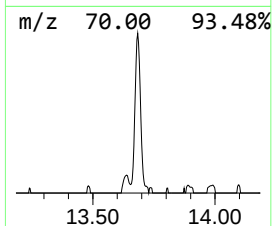
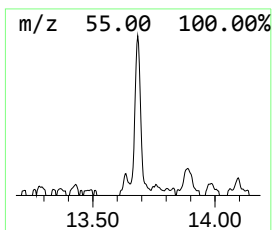
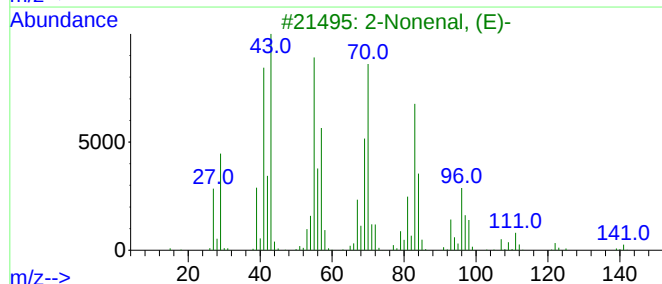
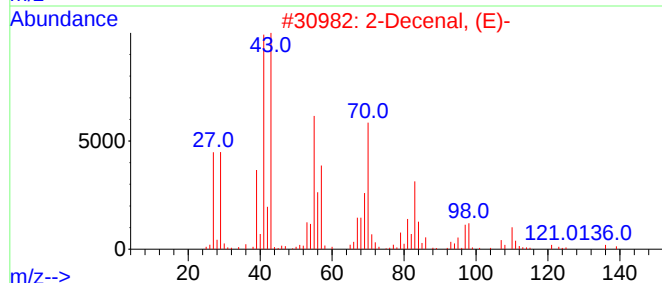
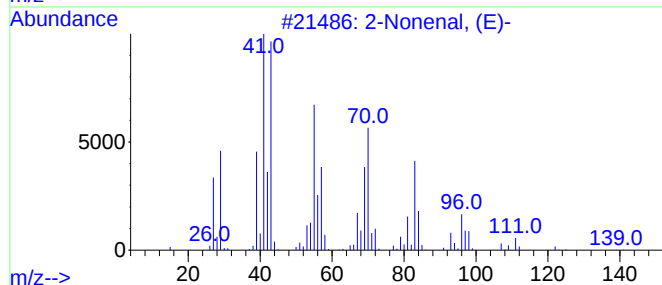
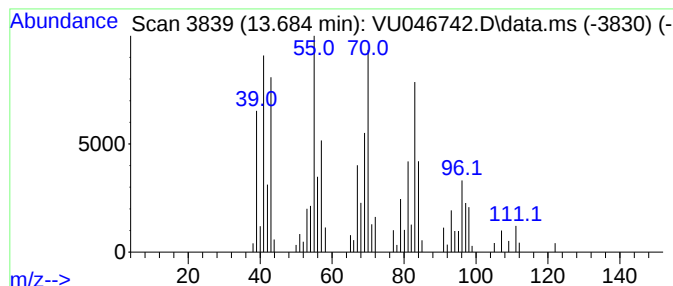
Instrument :
MSVOA_U
ClientSampleId :
BFXW3

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 10 2-Nonenal, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.684	1.14 ug/L	65717	1,4-Dichlorobenzene-d4	11.812	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonenal, (E)-	140	C9H16O	018829-56-6	64
2	2-Decenal, (E)-	154	C10H18O	003913-81-3	59
3	2-Nonenal, (E)-	140	C9H16O	018829-56-6	59
4	2-Decenal, (E)-	154	C10H18O	003913-81-3	53
5	2-Decenal, (Z)-	154	C10H18O	002497-25-8	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046742.D
Acq On : 12 Jan 2022 15:07
Operator : SY/MD
Sample : N1077-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW3

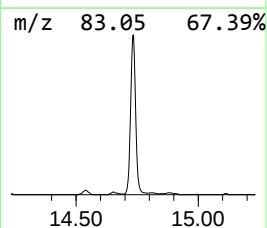
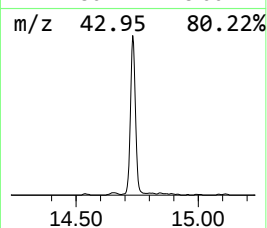
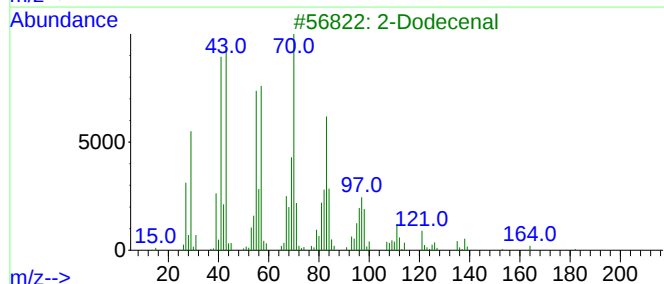
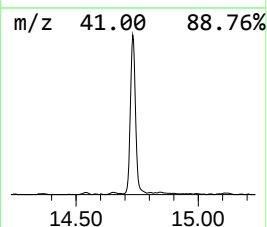
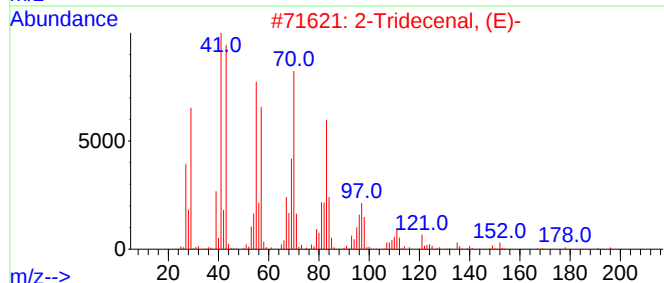
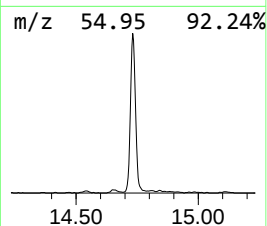
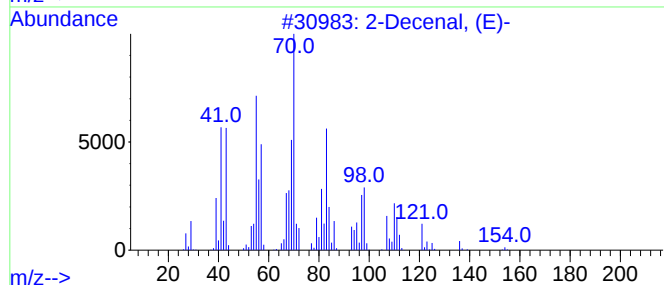
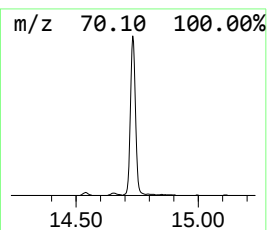
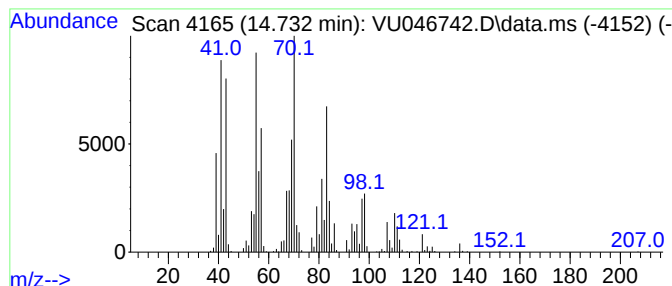
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2-Decenal, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.732	10.79 ug/L	619903	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decenal, (E)-	154	C10H18O	003913-81-3	91
2			2-Tridecenal, (E)-	196	C13H24O	007069-41-2	59
3			2-Dodecenal	182	C12H22O	004826-62-4	59
4			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	53
5			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046742.D
Acq On : 12 Jan 2022 15:07
Operator : SY/MD
Sample : N1077-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW3

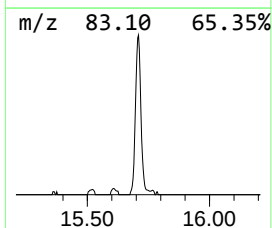
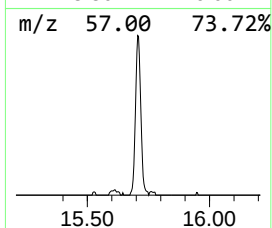
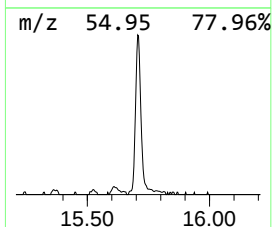
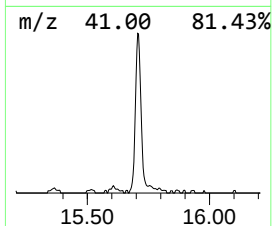
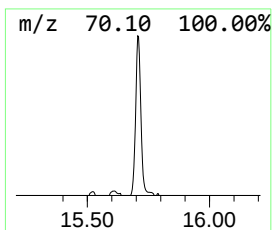
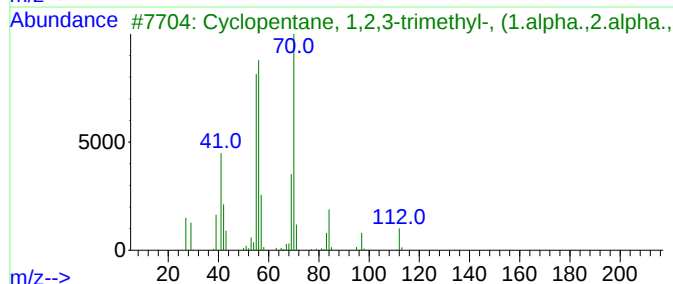
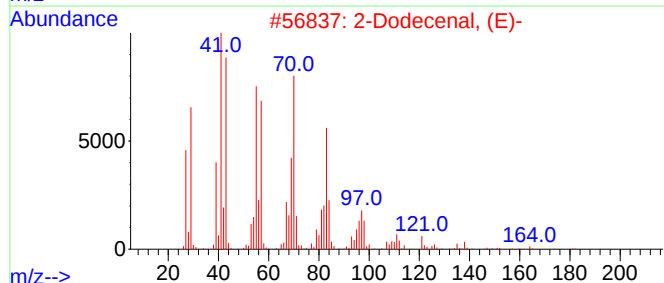
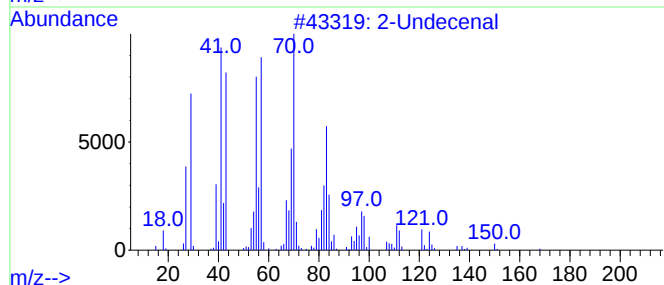
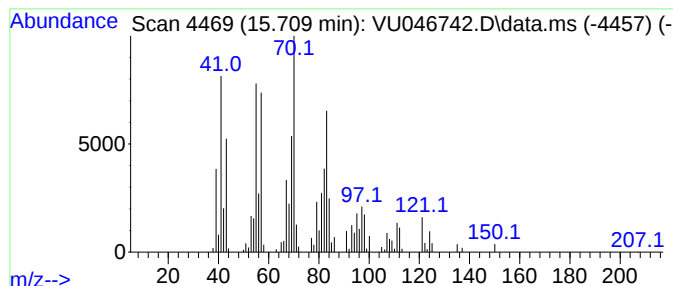
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 2-Undecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.709	2.60 ug/L	149272	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Undecenal	168	C11H20O	002463-77-6	80
2			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	43
3			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	38
4			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	30
5			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046742.D
Acq On : 12 Jan 2022 15:07
Operator : SY/MD
Sample : N1077-07
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW3

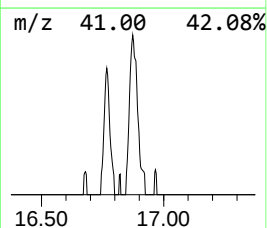
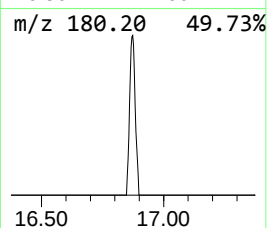
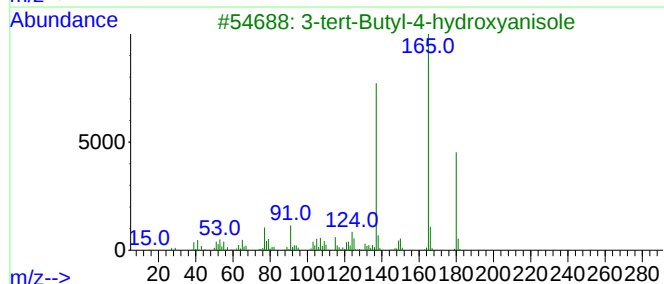
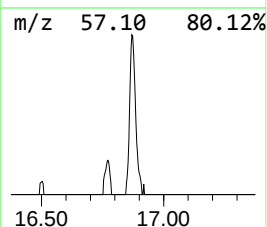
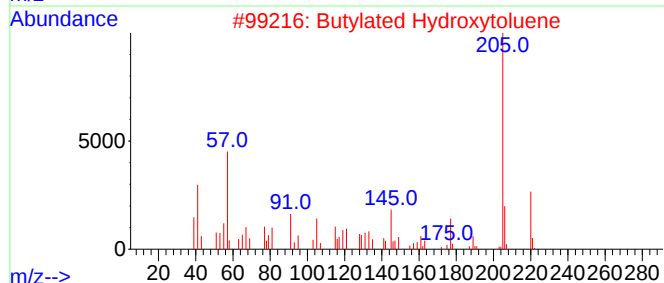
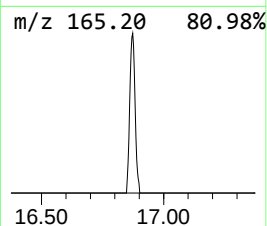
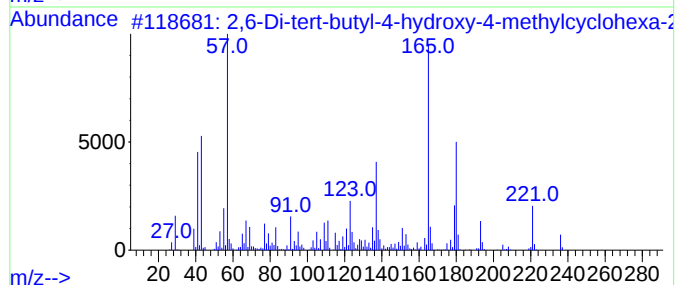
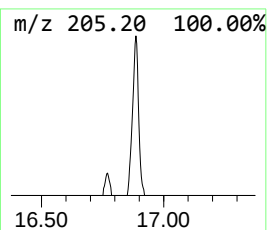
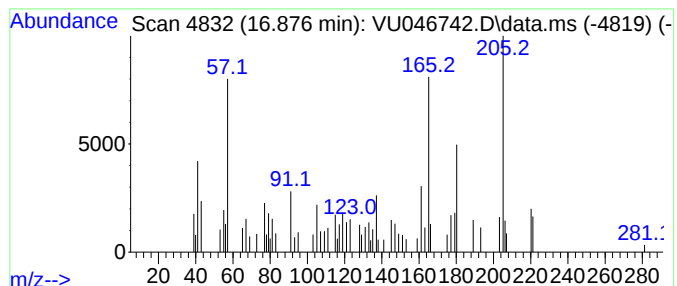
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 13 unknown-01 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.876	0.66 ug/L	38037	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Di-tert-butyl-4-hydroxy-4-me...	236	C15H24O2	010396-80-2	41		
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	38		
3	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	38		
4	Benzenethiol, 4-(1,1-dimethyleth...	180	C11H16S	015570-10-2	38		
5	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	38		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
 Data File : VU046742.D
 Acq On : 12 Jan 2022 15:07
 Operator : SY/MD
 Sample : N1077-07
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXW3

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
(DEL) Alkane: S...	2.211	3.0	ug/L	109014	1	6.272	181357	5.0
Pentanal	6.906	6.1	ug/L	222599	1	6.272	181357	5.0
Heptanal	10.349	3.8	ug/L	175087	2	9.423	232530	5.0
2-Heptenal, (E)-	11.298	1.9	ug/L	107401	3	11.812	287277	5.0
Octanal	11.690	6.7	ug/L	387228	3	11.812	287277	5.0
1-Hexanol, 2-et...	12.063	0.8	ug/L	45222	3	11.812	287277	5.0
2-Octenal, (E)-	12.545	5.7	ug/L	328617	3	11.812	287277	5.0
Nonanal	12.886	5.8	ug/L	331337	3	11.812	287277	5.0
2-Nonenal, (E)-	13.684	1.1	ug/L	65717	3	11.812	287277	5.0
2-Decenal, (E)-	14.732	10.8	ug/L	619903	3	11.812	287277	5.0
2-Undecenal	15.709	2.6	ug/L	149272	3	11.812	287277	5.0
unknown-01	16.876	0.7	ug/L	38037	3	11.812	287277	5.0