

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
 Data File : VU047029.D
 Acq On : 03 Feb 2022 18:14
 Operator : SY/MD
 Sample : N1348-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 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: VU047029.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	20	rVB	36467	35563	4.64%	0.547%
2	1.597	69	80	95	rBV3	69474	94656	12.35%	1.455%
3	1.700	104	112	121	rBV2	8160	14441	1.88%	0.222%
4	1.916	170	179	190	rBV	42800	57710	7.53%	0.887%
5	2.141	239	249	262	rVB	173274	255337	33.31%	3.926%
6	2.572	367	383	403	rVB4	117866	241560	31.51%	3.714%
7	3.877	772	789	808	rBV	52489	123907	16.16%	1.905%
8	4.465	960	972	986	rBV5	3301	10391	1.36%	0.160%
9	4.671	1016	1036	1083	rBV3	98876	294916	38.47%	4.534%
10	5.070	1143	1160	1184	rBV2	73875	187884	24.51%	2.889%
11	5.318	1225	1237	1248	rBV3	6853	13479	1.76%	0.207%
12	5.729	1342	1365	1395	rBV2	135150	355773	46.41%	5.470%
13	6.250	1512	1527	1546	rBV2	115773	223270	29.13%	3.433%
14	6.546	1605	1619	1641	rBV	263197	493612	64.39%	7.589%
15	6.694	1649	1665	1685	rBV	87477	170040	22.18%	2.614%
16	6.883	1713	1724	1743	rBV2	26796	56710	7.40%	0.872%
17	7.568	1926	1937	1953	rVB	39252	68317	8.91%	1.050%
18	7.899	2027	2040	2058	rBV	137549	259291	33.83%	3.987%
19	8.182	2118	2128	2141	rBV	23950	40426	5.27%	0.622%
20	8.555	2232	2244	2259	rBV	88492	152669	19.92%	2.347%
21	8.639	2259	2270	2304	rVV	162080	380576	49.65%	5.851%
22	8.787	2304	2316	2358	rVB	406714	766565	100.00%	11.786%
23	9.420	2500	2513	2539	rBV	192048	342843	44.72%	5.271%
24	10.346	2790	2801	2819	rBV2	65159	115089	15.01%	1.770%
25	10.758	2917	2929	2944	rBV	70378	114189	14.90%	1.756%
26	11.298	3089	3097	3105	rVV3	16380	26413	3.45%	0.406%
27	11.687	3206	3218	3239	rBV	124920	196293	25.61%	3.018%
28	11.812	3245	3257	3274	rVB	233277	371856	48.51%	5.717%
29	12.195	3363	3376	3389	rBV	152208	245816	32.07%	3.780%
30	12.542	3473	3484	3497	rBV4	27424	51932	6.77%	0.798%
31	12.886	3577	3591	3618	rBV	305476	468422	61.11%	7.202%
32	13.684	3831	3839	3849	rVB4	12503	17861	2.33%	0.275%
33	14.732	4153	4165	4183	rBV2	98097	156108	20.36%	2.400%
34	15.127	4280	4288	4299	rVB6	5949	9205	1.20%	0.142%
35	15.369	4352	4363	4380	rBV	24429	40167	5.24%	0.618%
36	15.706	4459	4468	4483	rBV2	26934	42768	5.58%	0.658%

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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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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

37	16.886	4825	4835	4846	rVB6	4537	7863	1.03%	0.121%
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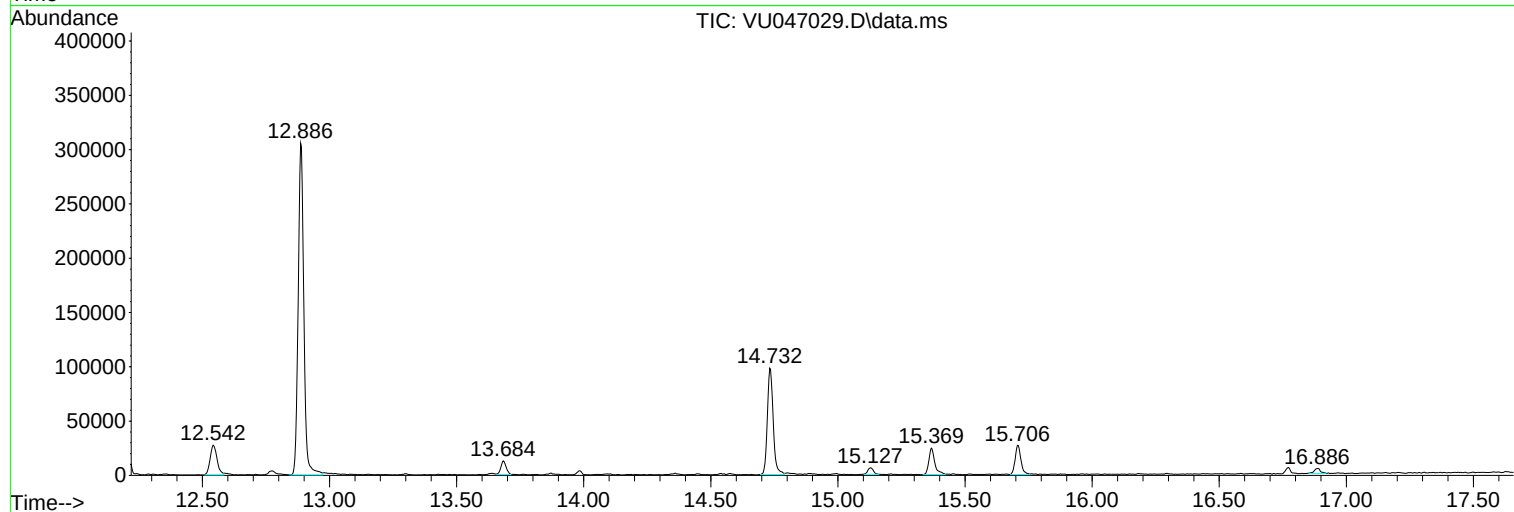
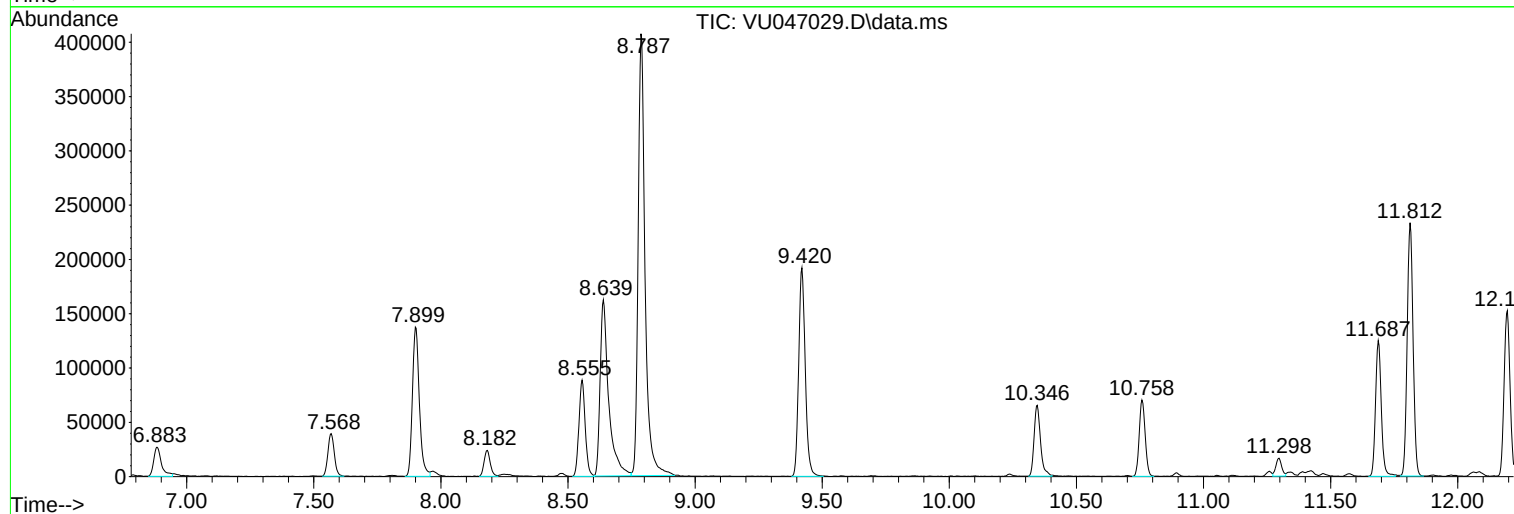
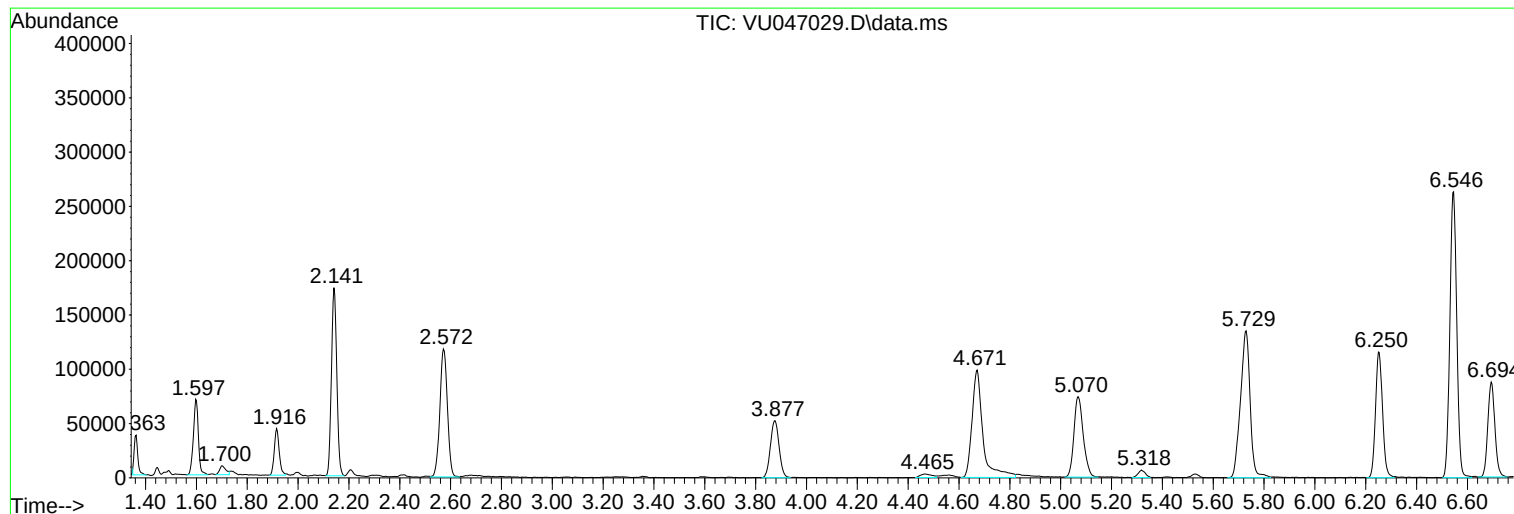
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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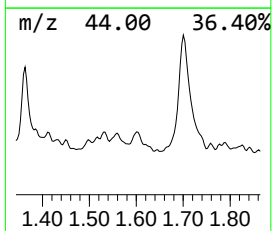
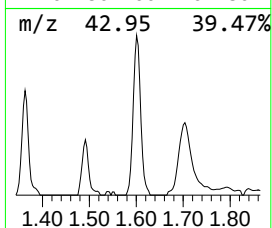
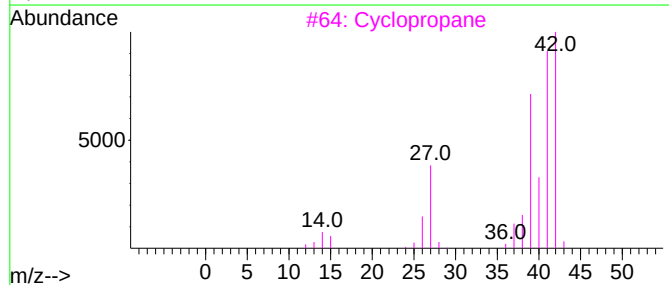
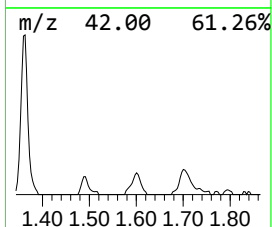
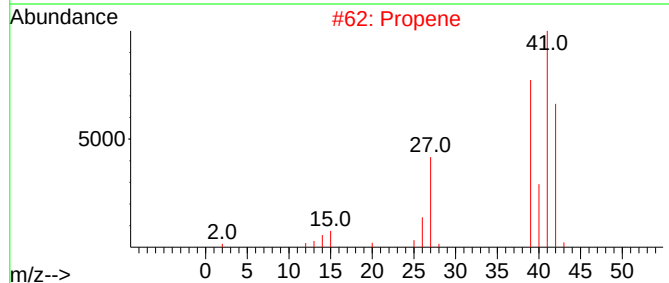
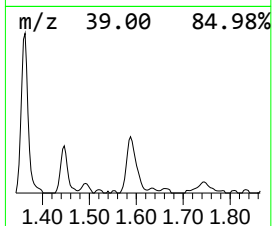
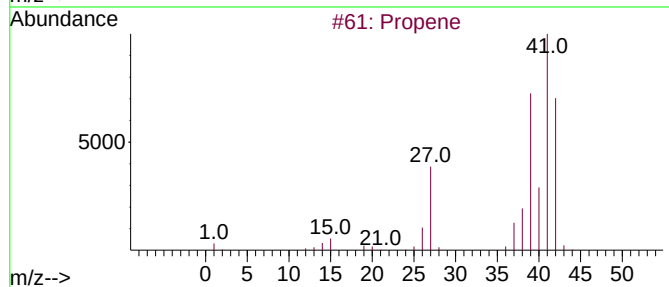
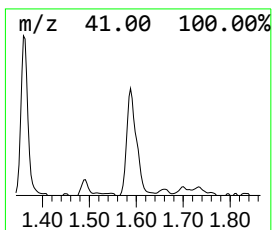
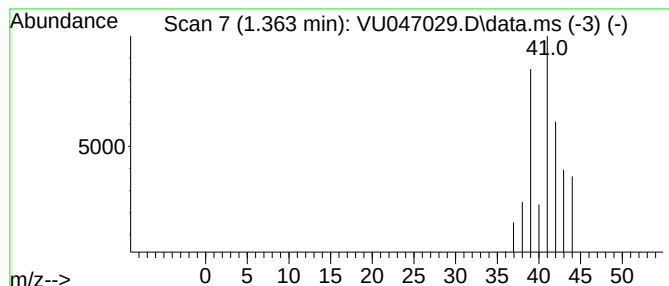
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.363	0.80 ug/L	35563	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	64
2			Propene	42	C3H6	000115-07-1	42
3			Cyclopropane	42	C3H6	000075-19-4	7
4			Cyclopropane	42	C3H6	000075-19-4	4
5			Cyclopropene	40	C3H4	002781-85-3	4



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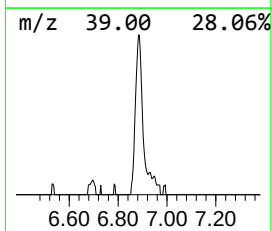
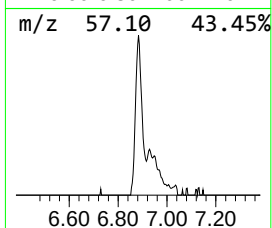
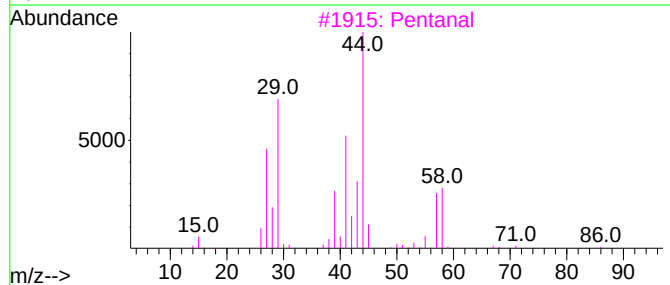
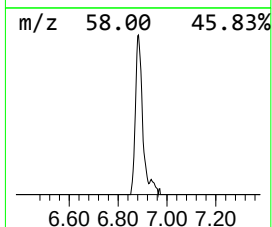
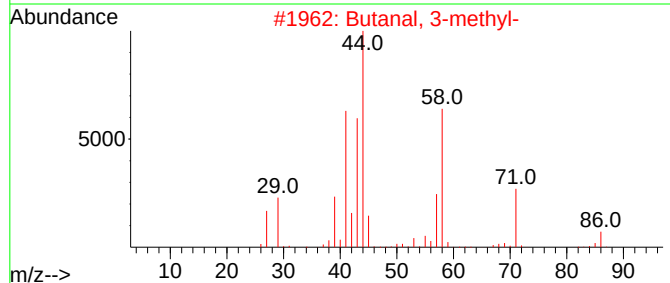
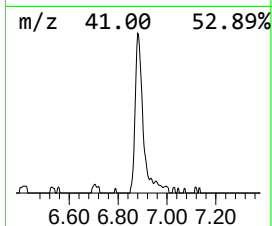
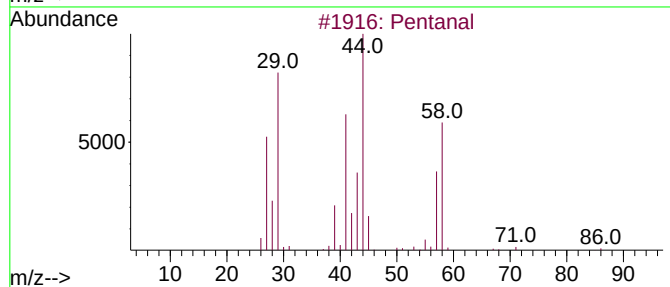
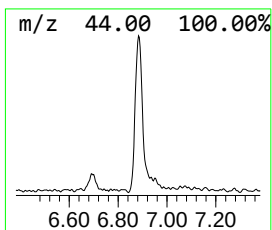
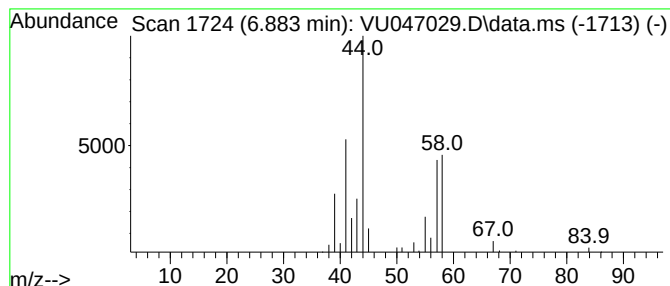
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	1.27 ug/L	56710	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	80
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	78
3			Pentanal	86	C5H10O	000110-62-3	53
4			Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	28



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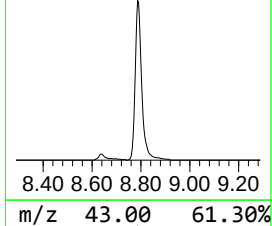
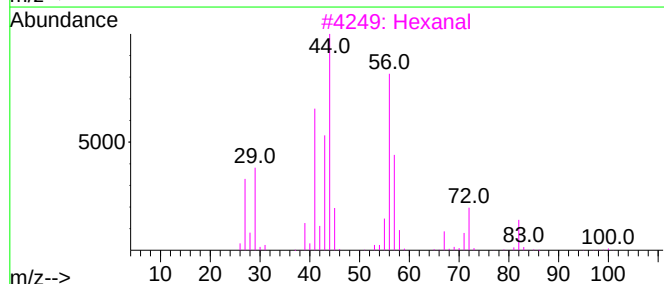
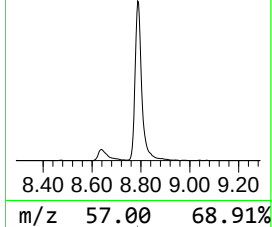
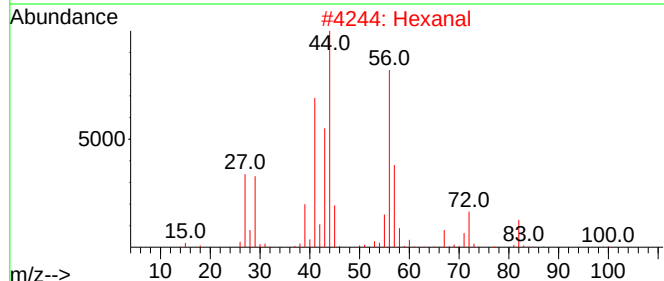
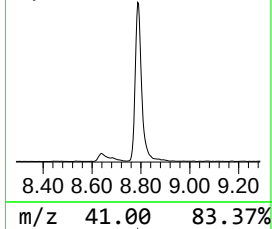
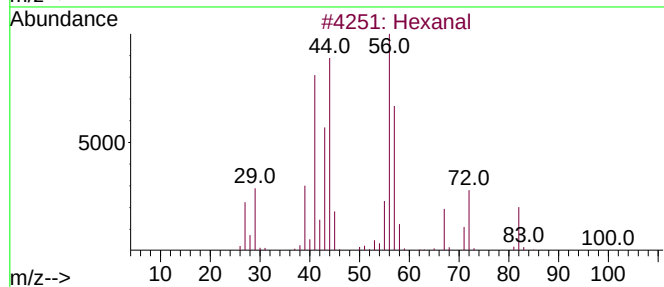
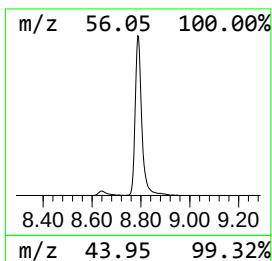
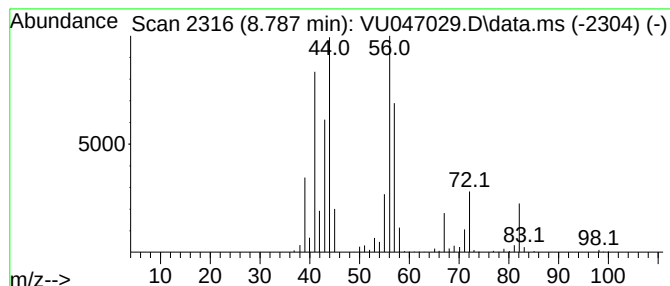
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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	11.18 ug/L	766565	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	90
4	Hexanal			100	C6H12O	000066-25-1	86
5	Hexanal			100	C6H12O	000066-25-1	83



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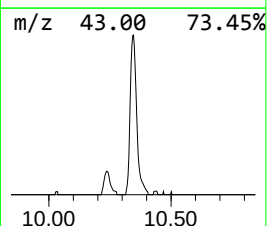
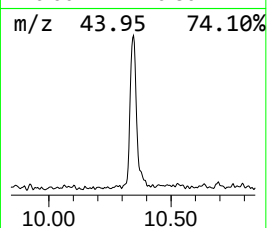
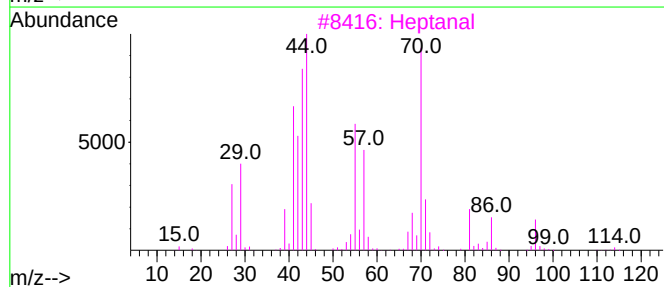
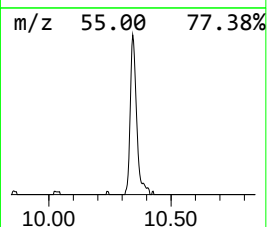
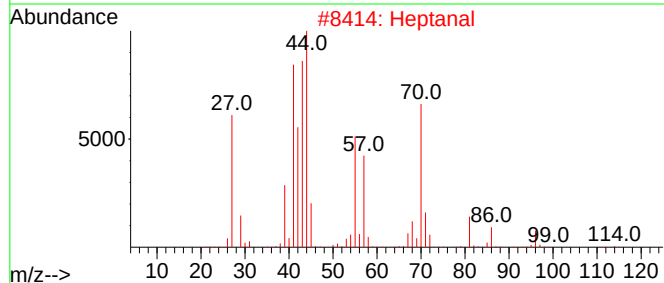
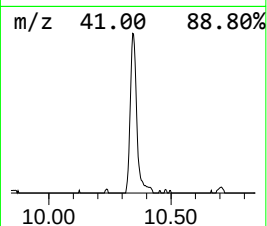
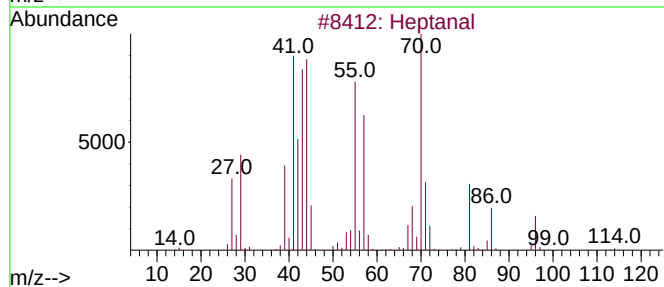
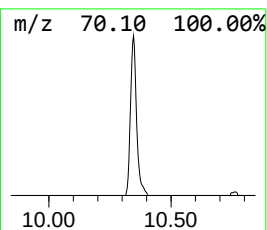
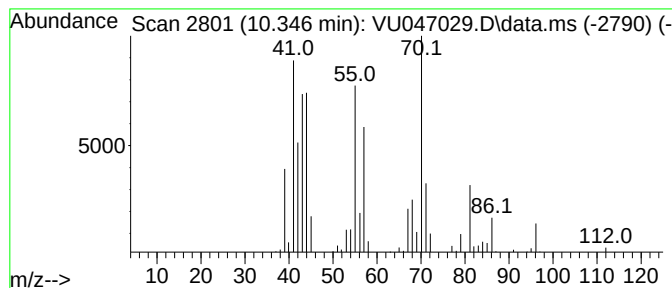
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Heptanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.346	1.68 ug/L	115089	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	96
2			Heptanal	114	C7H14O	000111-71-7	93
3			Heptanal	114	C7H14O	000111-71-7	74
4			Heptanal	114	C7H14O	000111-71-7	50
5			Heptanal	114	C7H14O	000111-71-7	38



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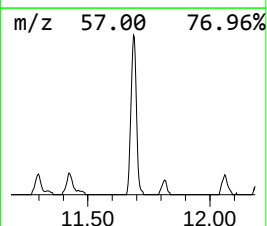
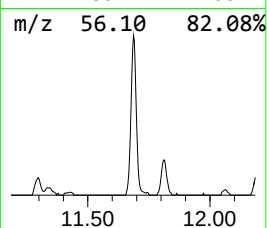
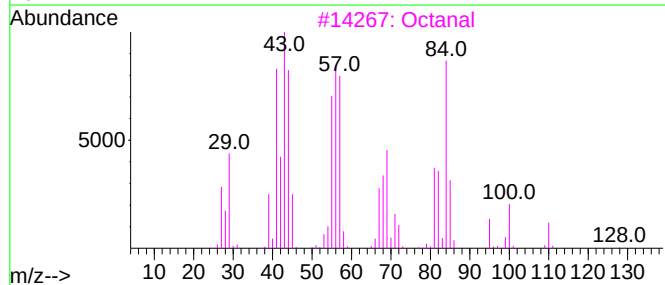
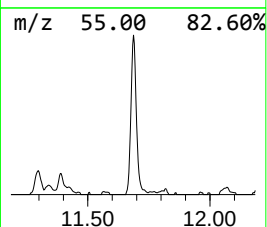
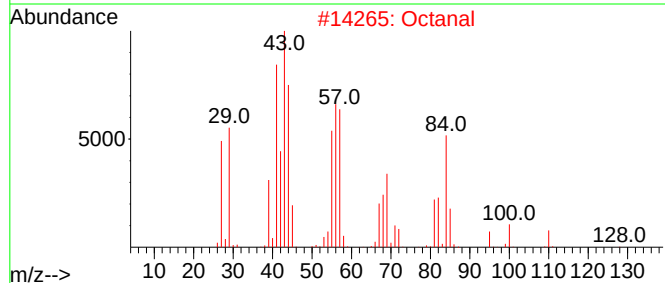
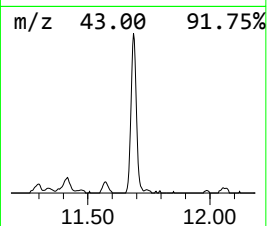
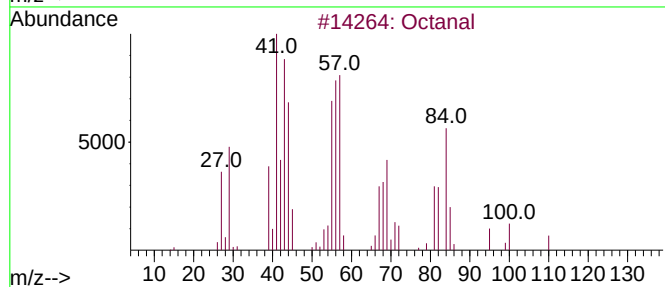
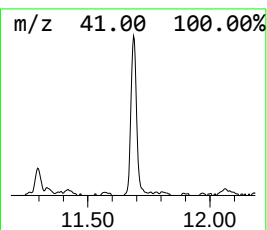
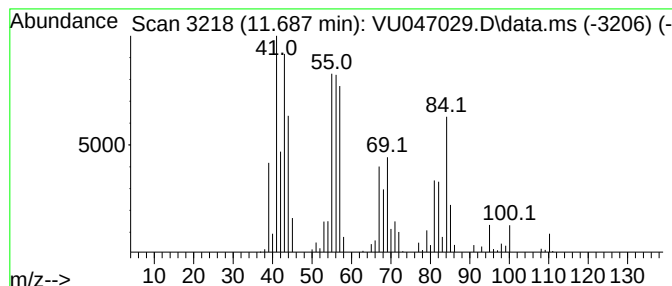
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	2.64 ug/L	196293	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	87
2	Octanal			128	C8H16O	000124-13-0	86
3	Octanal			128	C8H16O	000124-13-0	58
4	Octanal			128	C8H16O	000124-13-0	50
5	1-Pentene, 3-methyl-			84	C6H12	000760-20-3	46



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Operator : SY/MD
Sample : N1348-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX9

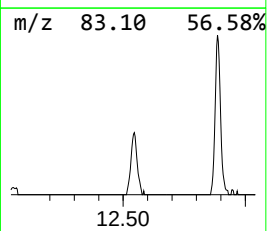
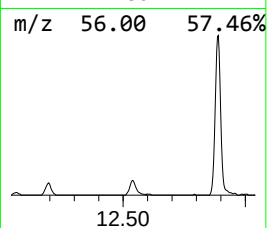
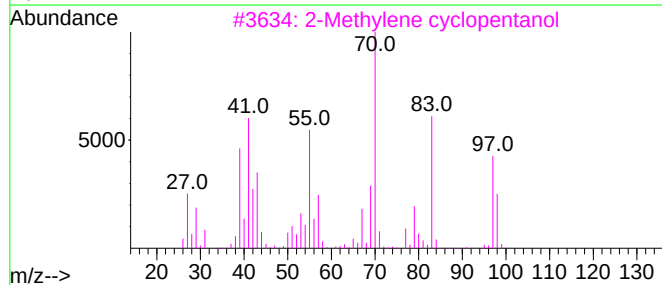
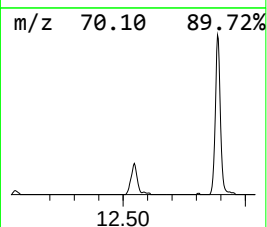
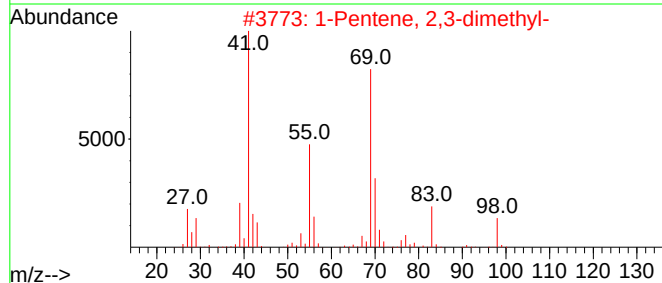
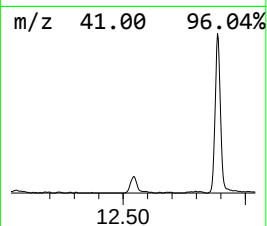
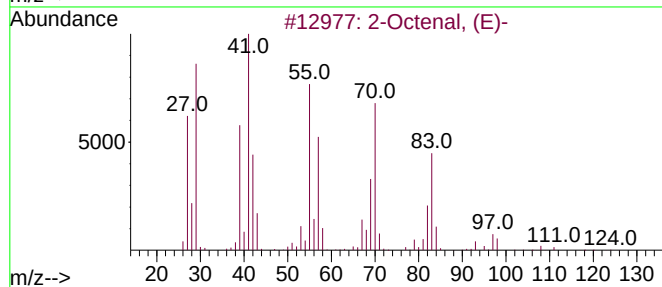
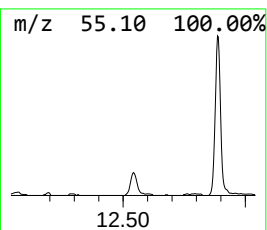
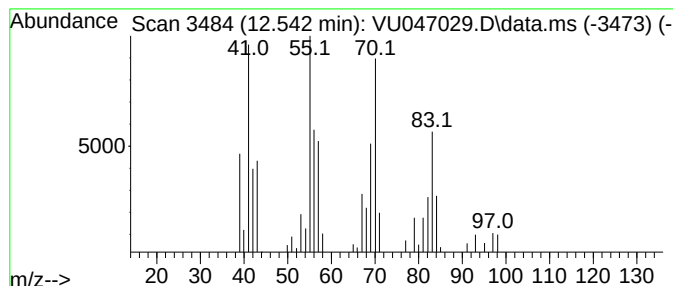
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 2-Octenal, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.542	0.70 ug/L	51932	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octenal, (E)-	126	C8H14O	002548-87-0	53
2			1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	50
3			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	43
4			1,5-Diazabicyclo[3.1.0]hexane	84	C4H8N2	013090-31-8	38
5			2-(Oxolan-3-yl)ethanol	116	C6H12O2	1050496-48-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047029.D
Acq On : 03 Feb 2022 18:14
Operator : SY/MD
Sample : N1348-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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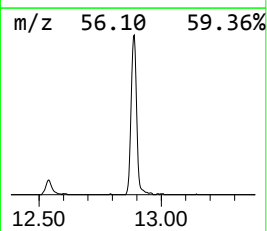
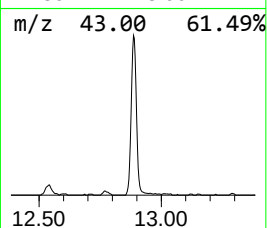
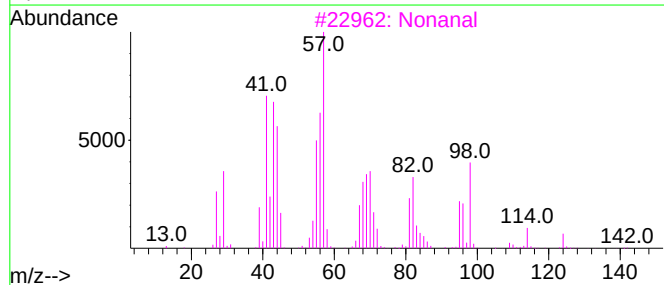
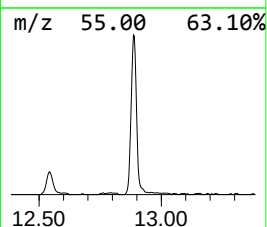
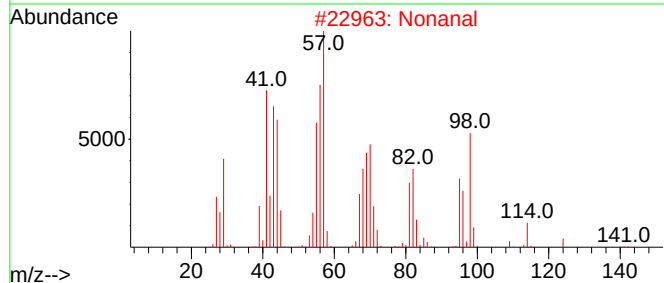
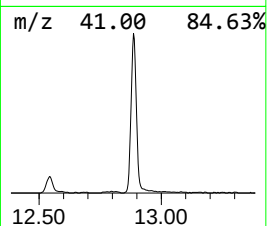
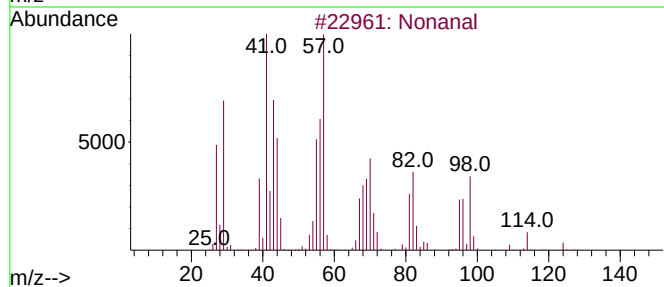
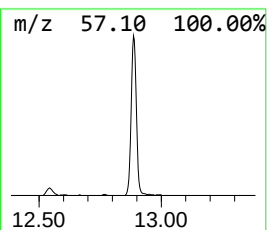
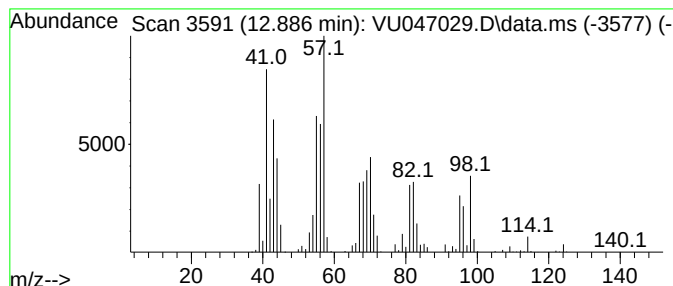
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	6.30 ug/L	468422	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	90
3			Nonanal	142	C9H18O	000124-19-6	72
4			Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	30
5			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047029.D
Acq On : 03 Feb 2022 18:14
Operator : SY/MD
Sample : N1348-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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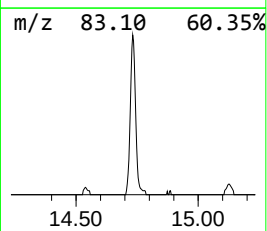
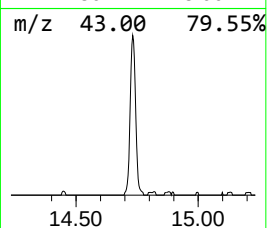
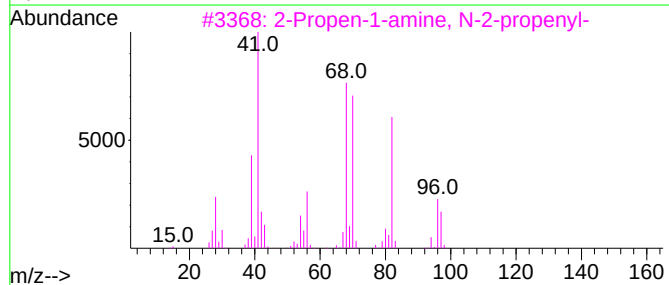
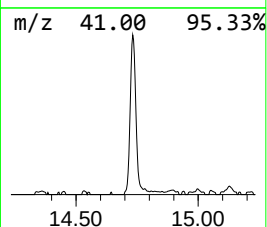
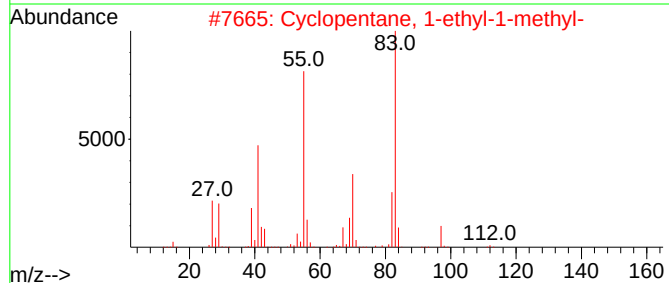
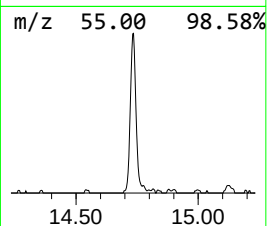
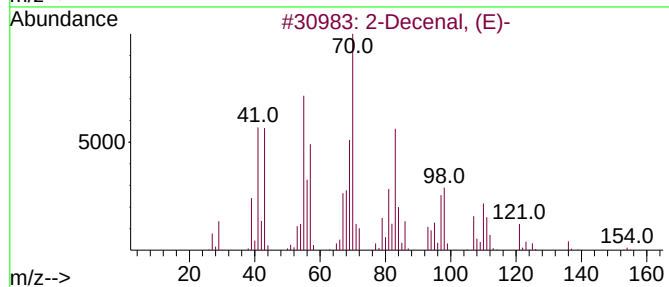
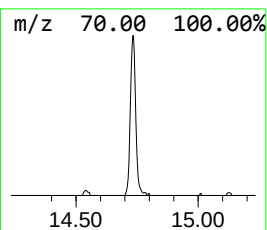
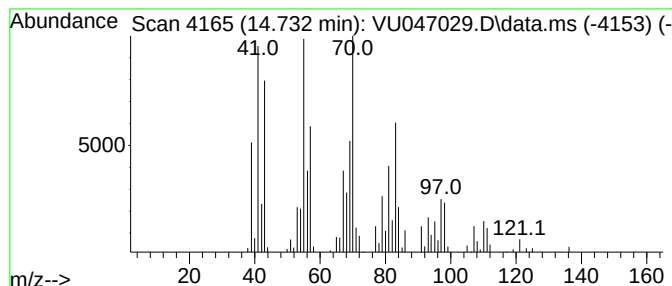
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 2-Decenal, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.732	2.10 ug/L	156108	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decenal, (E)-	154	C10H18O	003913-81-3	58
2			Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	49
3			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	43
4			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	43
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047029.D
Acq On : 03 Feb 2022 18:14
Operator : SY/MD
Sample : N1348-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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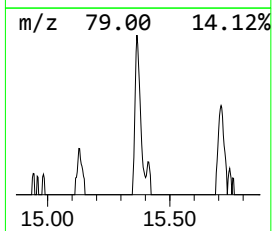
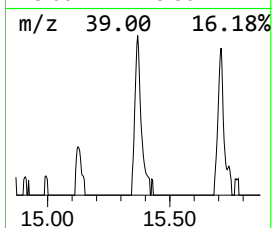
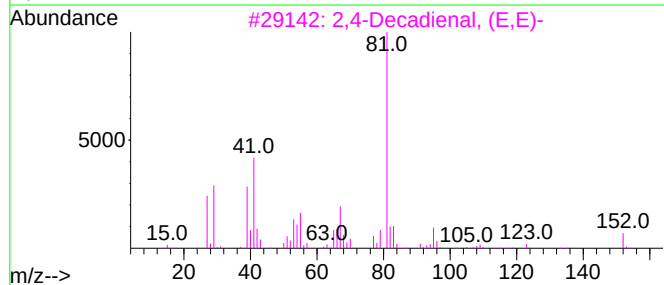
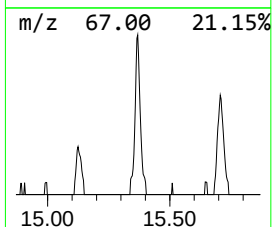
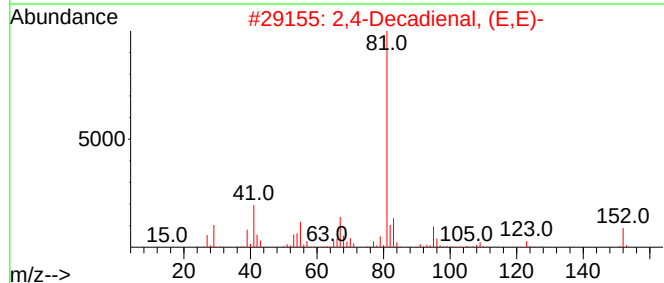
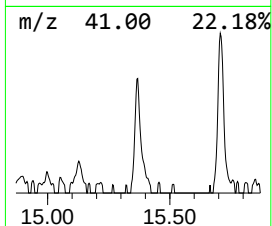
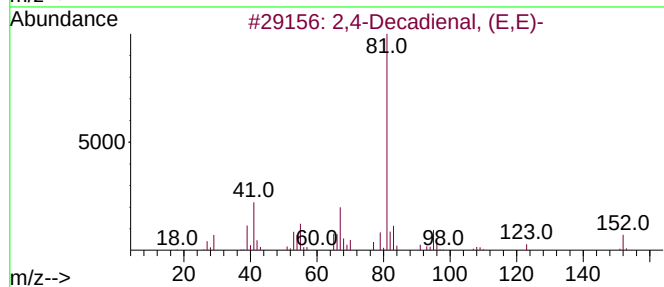
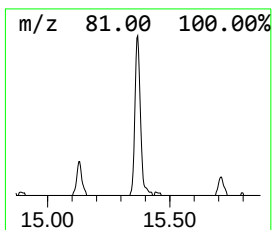
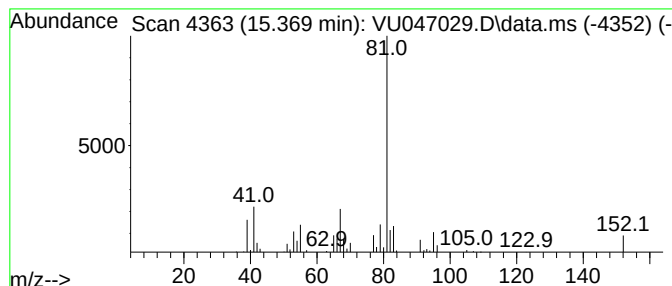
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 2,4-Decadienal, (E,E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.369	0.54 ug/L	40167	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	90
2			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	90
3			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	83
4			2,4-Decadienal, (E,E)-	152	C10H16O	025152-84-5	83
5			2,4-Nonadienal, (E,E)-	138	C9H14O	005910-87-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047029.D
Acq On : 03 Feb 2022 18:14
Operator : SY/MD
Sample : N1348-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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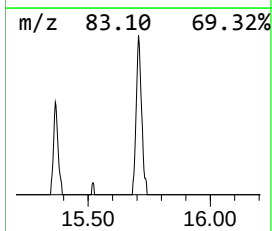
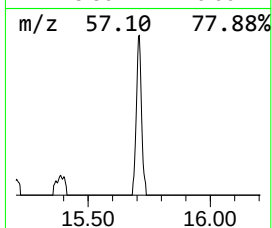
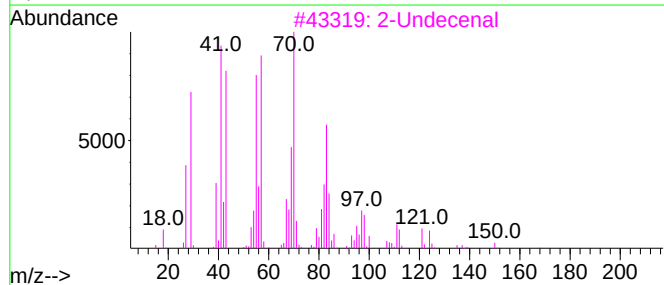
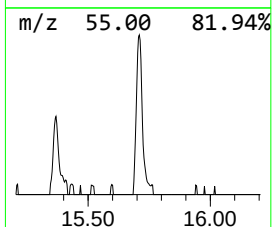
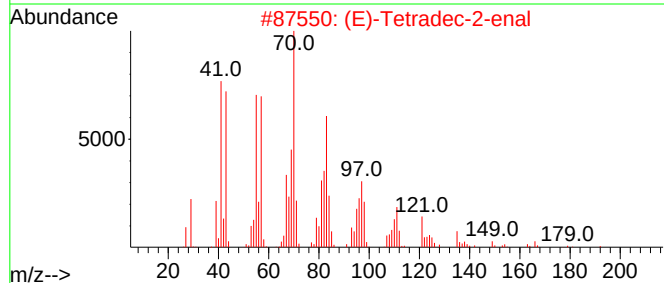
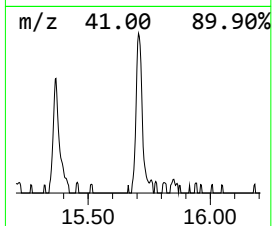
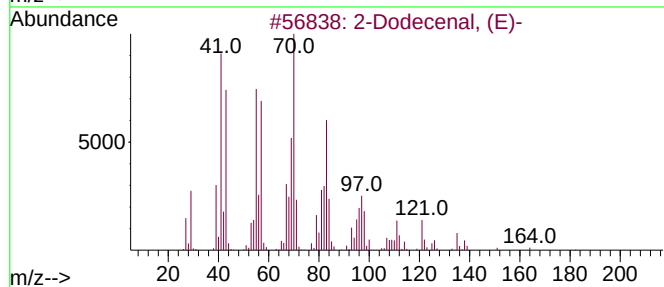
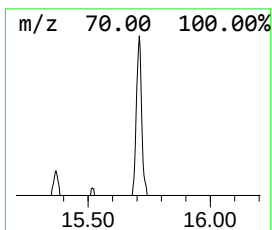
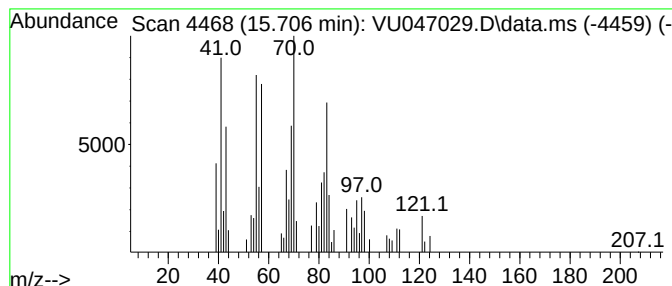
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2-Dodecenal, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.706	0.58 ug/L	42768	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	80
2			(E)-Tetradec-2-enal	210	C14H26O	051534-36-2	80
3			2-Undecenal	168	C11H20O	002463-77-6	80
4			4-Methyl-cyclohex-2-en-1-ol	112	C7H12O	1000144-17-5	35
5			1-Hexadecanol	242	C16H34O	036653-82-4	30



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047029.D
Acq On : 03 Feb 2022 18:14
Operator : SY/MD
Sample : N1348-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 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
(DEL) Alkane: S...	1.363	0.8	ug/L	35563	1	6.250	223270	5.0
Pentanal	6.883	1.3	ug/L	56710	1	6.250	223270	5.0
Hexanal	8.787	11.2	ug/L	766565	2	9.420	342843	5.0
Heptanal	10.346	1.7	ug/L	115089	2	9.420	342843	5.0
Octanal	11.687	2.6	ug/L	196293	3	11.813	371856	5.0
2-Octenal, (E)-	12.542	0.7	ug/L	51932	3	11.813	371856	5.0
Nonanal	12.886	6.3	ug/L	468422	3	11.813	371856	5.0
2-Decenal, (E)-	14.732	2.1	ug/L	156108	3	11.813	371856	5.0
2,4-Decadienal,...	15.369	0.5	ug/L	40167	3	11.813	371856	5.0
2-Dodecenal, (E)-	15.706	0.6	ug/L	42768	3	11.813	371856	5.0