

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
 Data File : VU046798.D
 Acq On : 19 Jan 2022 15:00
 Operator : SY/MD
 Sample : N1194-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX2

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: VU046798.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	19	rVB	63805	63446	6.56%	0.843%
2	1.475	36	42	53	rVB	56749	60062	6.21%	0.798%
3	1.600	70	81	97	rBV2	84947	124890	12.92%	1.659%
4	1.732	117	122	135	rVB5	5663	10049	1.04%	0.133%
5	1.919	170	180	198	rBV	54317	76455	7.91%	1.015%
6	2.211	263	271	281	rBV3	6030	10478	1.08%	0.139%
7	2.578	366	385	400	rBV3	169147	344880	35.67%	4.580%
8	3.874	748	788	813	rBV	169832	418441	43.28%	5.557%
9	4.652	1013	1030	1096	rBV2	59378	283442	29.32%	3.764%
10	5.067	1143	1159	1182	rBV2	96005	218090	22.56%	2.896%
11	5.321	1224	1238	1256	rVB4	19764	43225	4.47%	0.574%
12	5.729	1344	1365	1395	rBV2	199080	524970	54.30%	6.972%
13	6.250	1514	1527	1551	rBV	136089	254710	26.34%	3.383%
14	6.542	1601	1618	1645	rBV	509243	966877	100.00%	12.841%
15	6.694	1652	1665	1686	rVB	121504	236240	24.43%	3.137%
16	6.883	1710	1724	1755	rBV2	18591	43573	4.51%	0.579%
17	7.568	1925	1937	1951	rBV	63818	110304	11.41%	1.465%
18	7.899	2026	2040	2056	rBV	249204	426072	44.07%	5.658%
19	7.970	2056	2062	2073	rVB	5968	9961	1.03%	0.132%
20	8.182	2115	2128	2143	rBV	38670	66133	6.84%	0.878%
21	8.555	2233	2244	2256	rBV2	17434	28367	2.93%	0.377%
22	8.636	2256	2269	2305	rBV	391241	717212	74.18%	9.525%
23	8.787	2305	2316	2347	rVB	197289	355509	36.77%	4.721%
24	9.420	2499	2513	2533	rBV	207233	346423	35.83%	4.601%
25	10.343	2789	2800	2814	rBV2	42765	68411	7.08%	0.909%
26	10.758	2916	2929	2947	rVB	117763	187240	19.37%	2.487%
27	11.259	3074	3085	3091	rBV2	14997	21807	2.26%	0.290%
28	11.295	3091	3096	3107	rVB6	7420	12191	1.26%	0.162%
29	11.687	3207	3218	3236	rBV	104988	160971	16.65%	2.138%
30	11.812	3245	3257	3275	rBV	252034	400141	41.38%	5.314%
31	12.195	3363	3376	3389	rBV	248233	403030	41.68%	5.352%
32	12.545	3474	3485	3497	rBV5	10295	18663	1.93%	0.248%
33	12.889	3580	3592	3618	rBV	327181	484795	50.14%	6.438%
34	14.732	4156	4165	4176	rBV3	21799	32834	3.40%	0.436%

Sum of corrected areas: 7529892

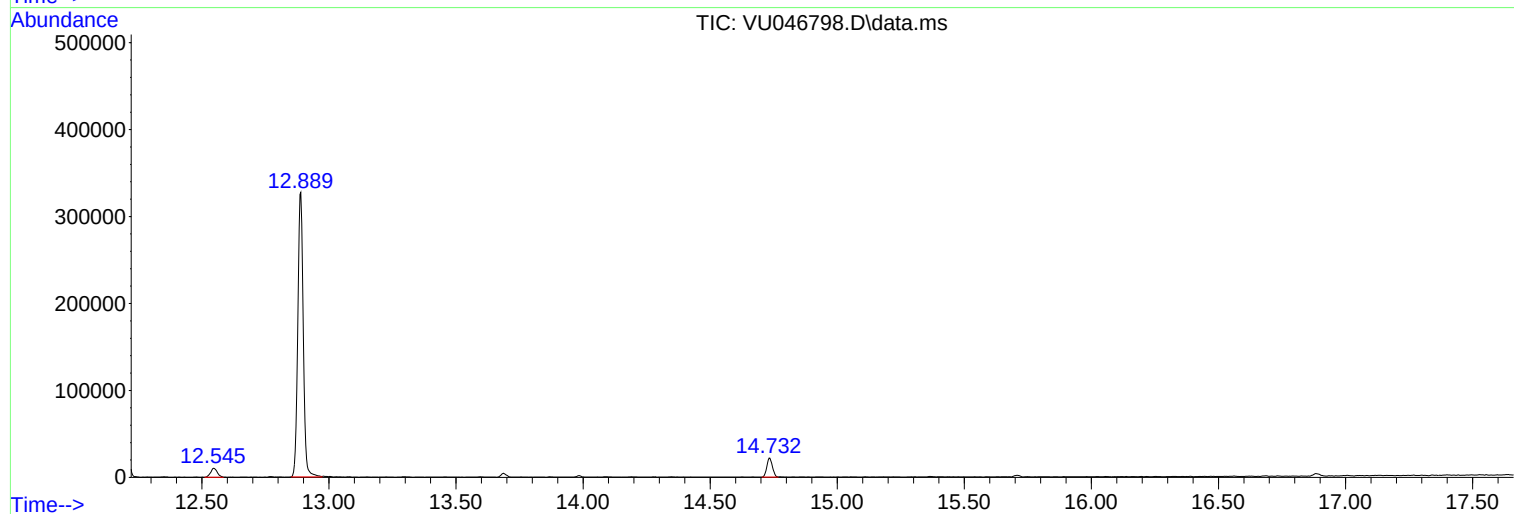
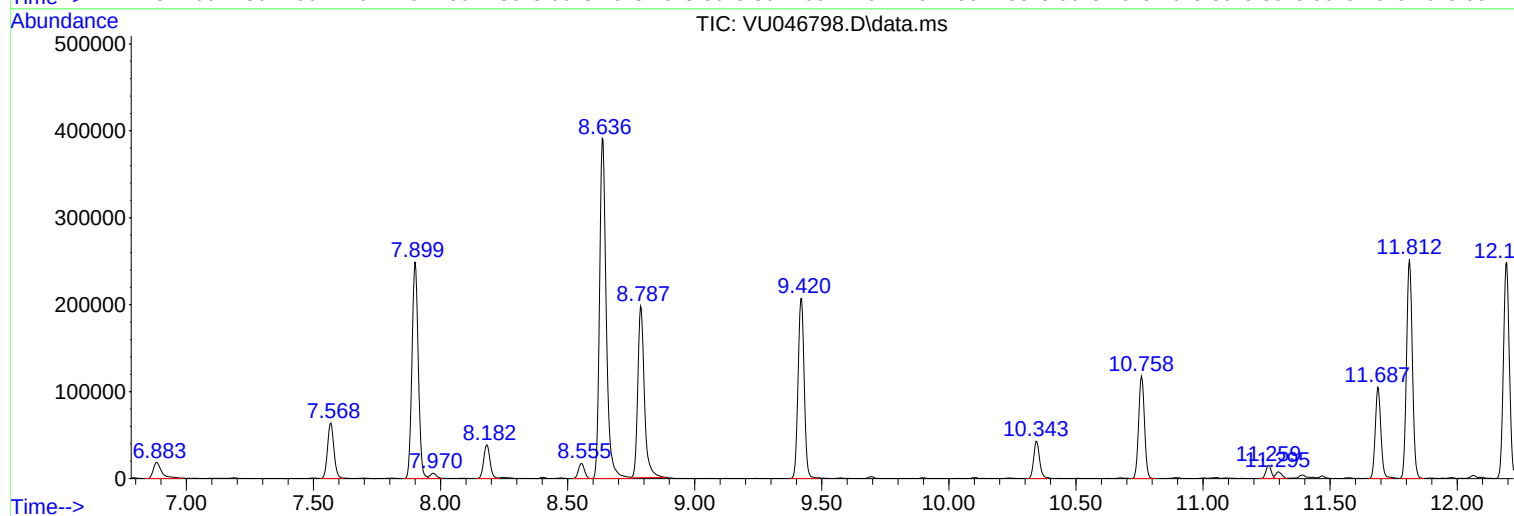
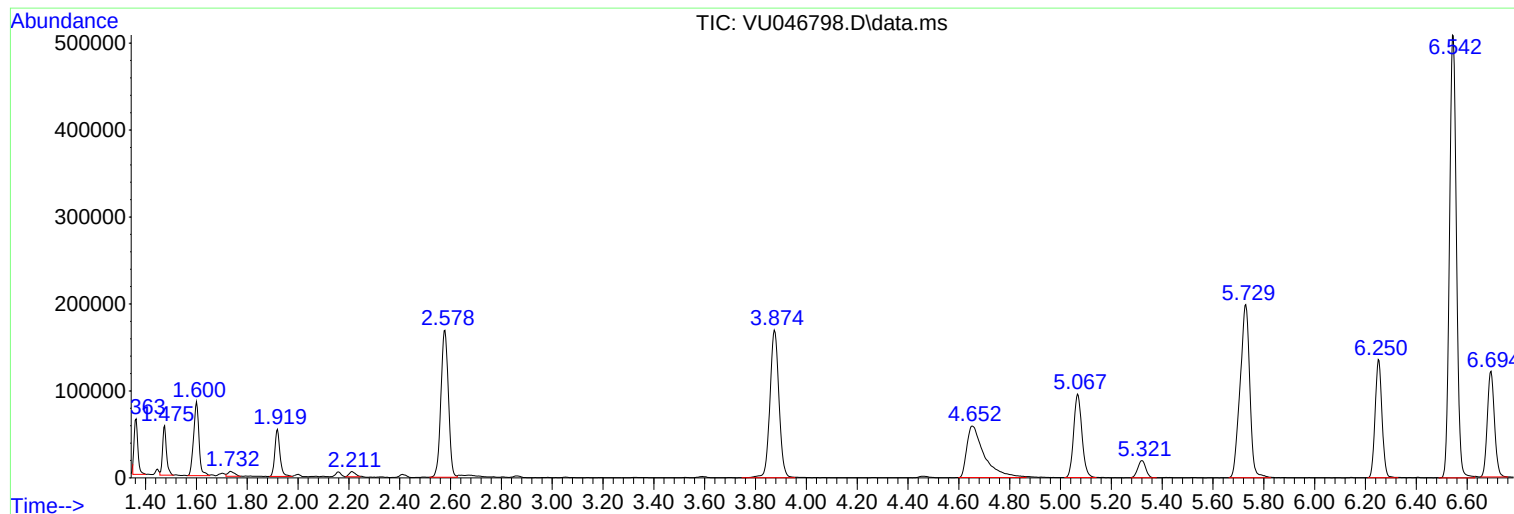
Instrument :
MSVOA_U
ClientSampleId :
BFXX2

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BFXX2

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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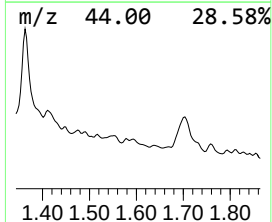
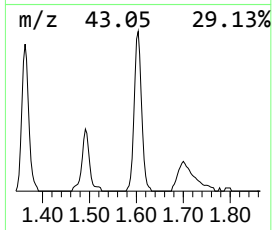
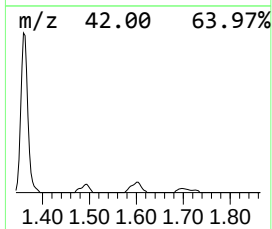
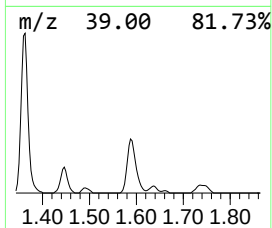
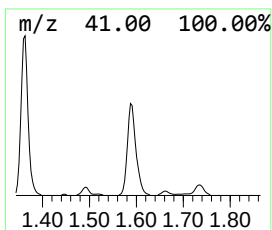
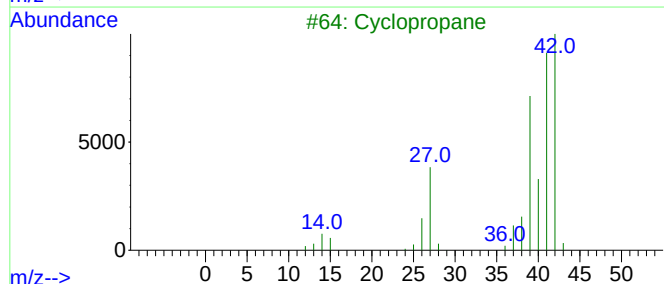
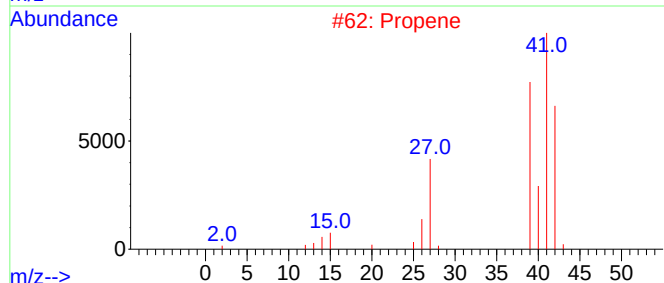
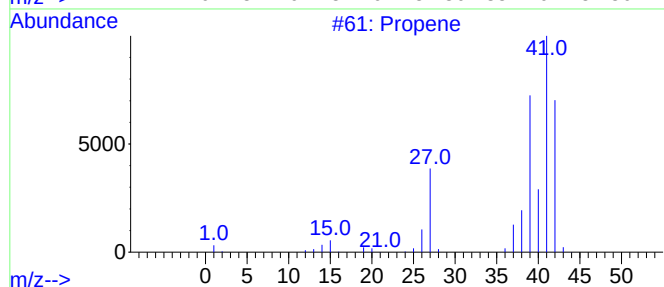
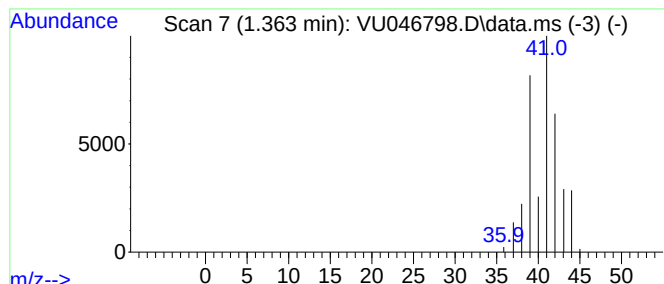
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.363	1.25 ug/L	63446	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Propene	42	C3H6	000115-07-1	42
3			Cyclopropane	42	C3H6	000075-19-4	9
4			Cyclopropene	40	C3H4	002781-85-3	9
5			Cyclopropane	42	C3H6	000075-19-4	7



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ALS Vial : 9 Sample Multiplier: 1

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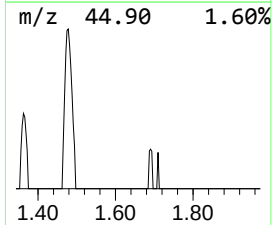
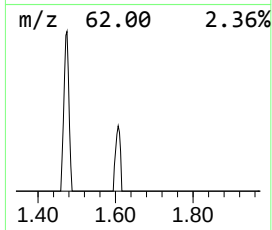
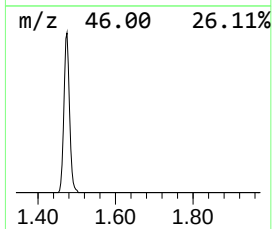
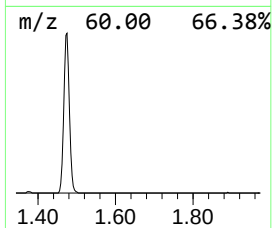
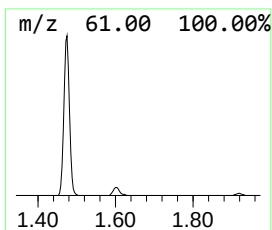
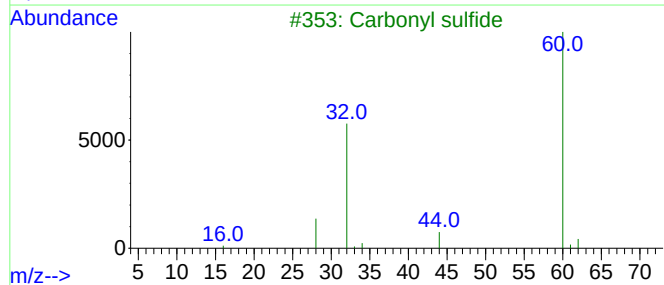
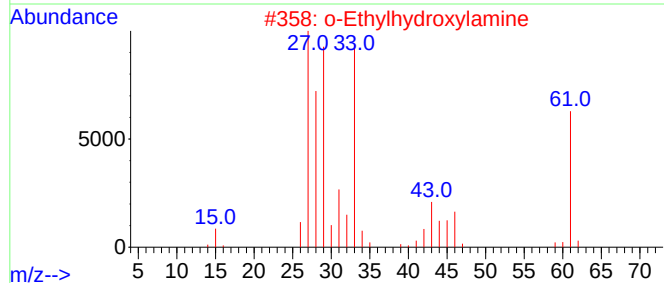
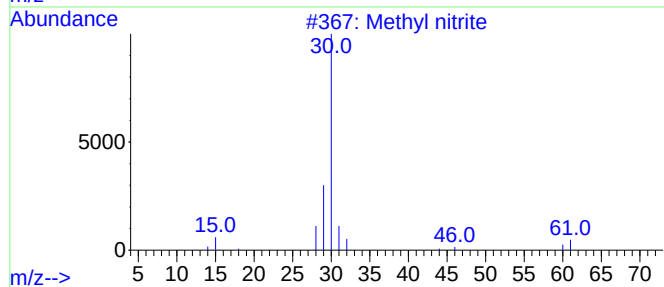
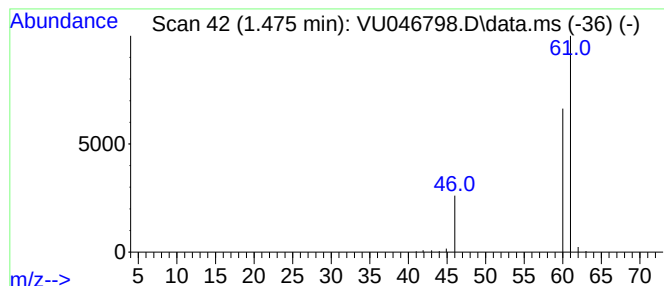
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	1.18 ug/L	60062	1,4-Difluorobenzene	6.250

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			Carbonyl sulfide	60	COS	000463-58-1	4
4			Thiirane	60	C2H4S	000420-12-2	4
5			Carbonyl sulfide	60	COS	000463-58-1	4



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ALS Vial : 9 Sample Multiplier: 1

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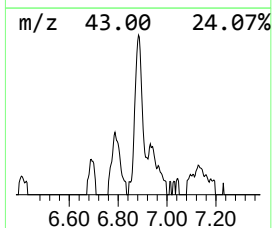
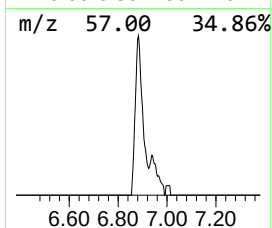
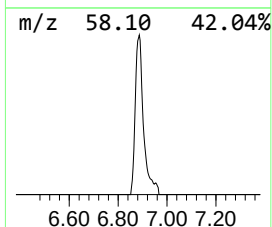
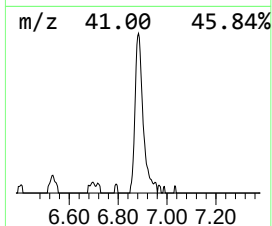
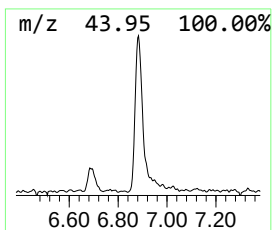
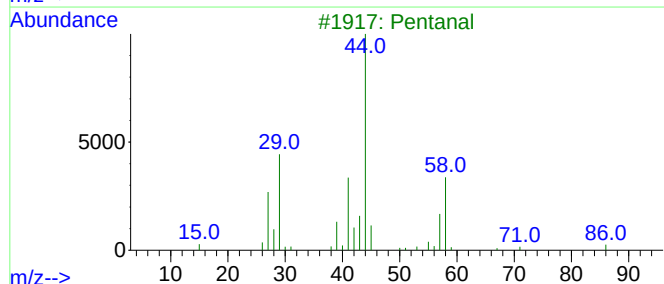
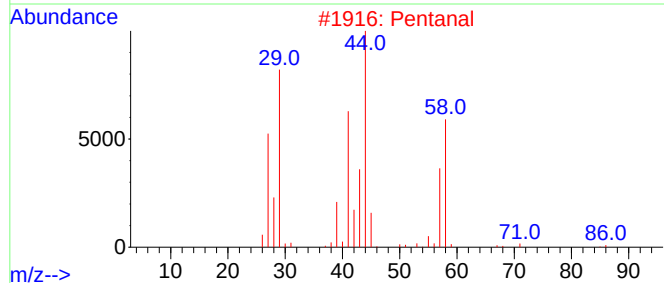
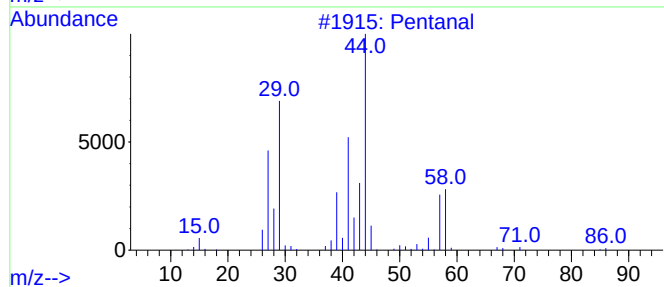
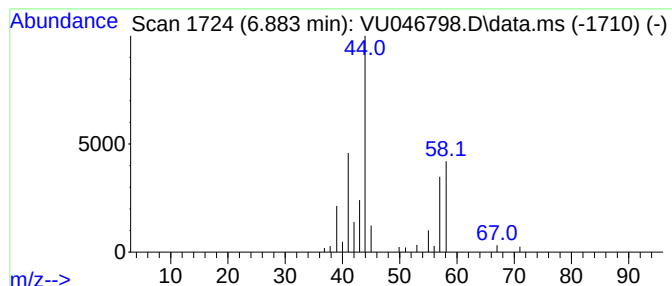
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Pentanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	0.86 ug/L	43573	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	83
2	Pentanal			86	C5H10O	000110-62-3	83
3	Pentanal			86	C5H10O	000110-62-3	78
4	Cyclopropyl carbinol			72	C4H8O	002516-33-8	28
5	1-Octadecanamine, N-methyl-			283	C19H41N	002439-55-6	9



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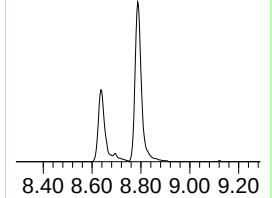
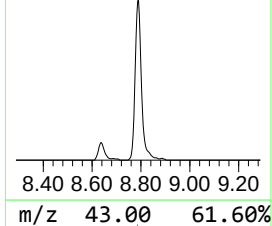
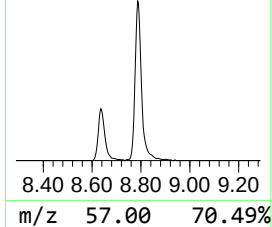
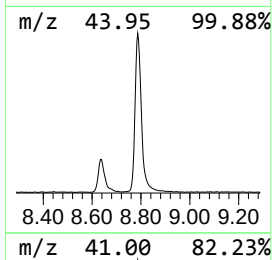
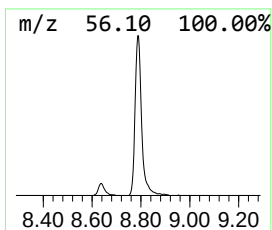
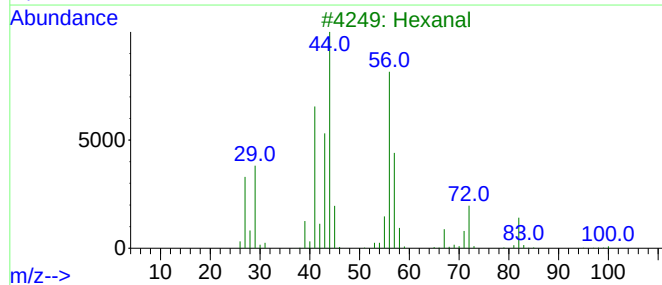
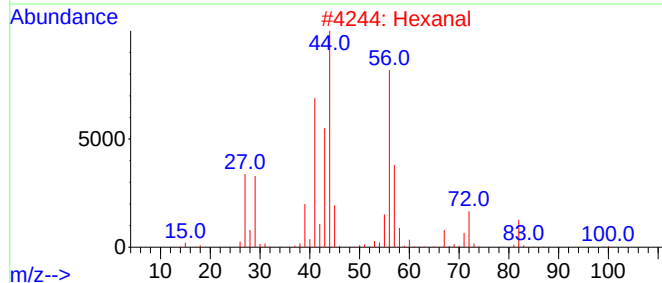
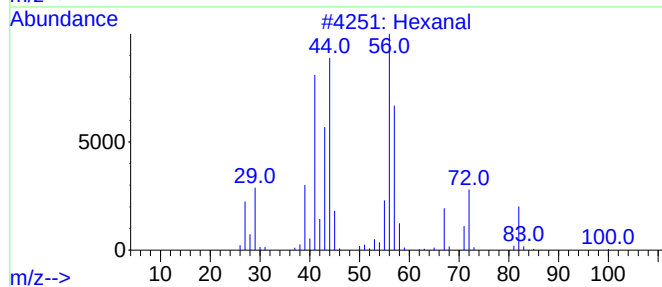
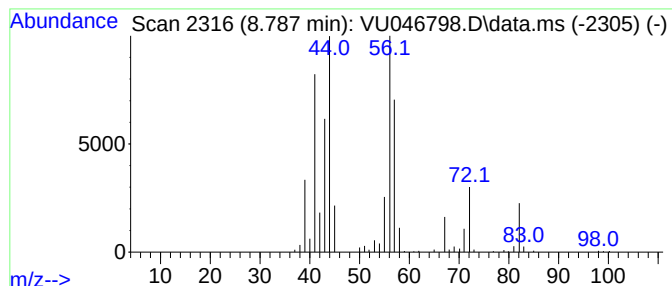
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	5.13 ug/L	355509	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	95
2	Hexanal			100	C6H12O	000066-25-1	94
3	Hexanal			100	C6H12O	000066-25-1	91
4	Hexanal			100	C6H12O	000066-25-1	90
5	Hexanal			100	C6H12O	000066-25-1	83



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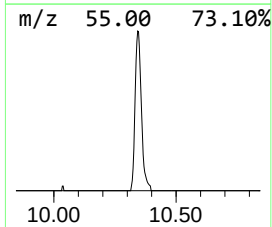
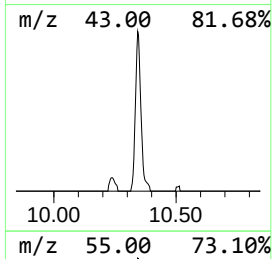
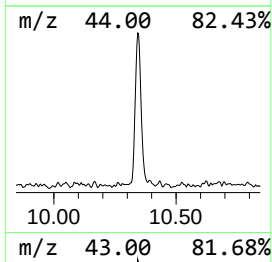
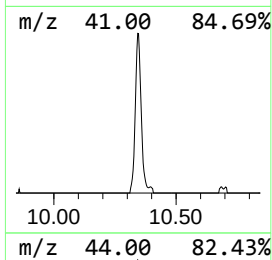
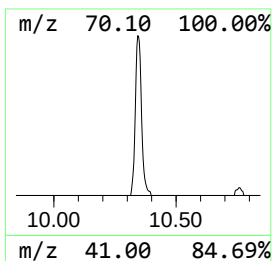
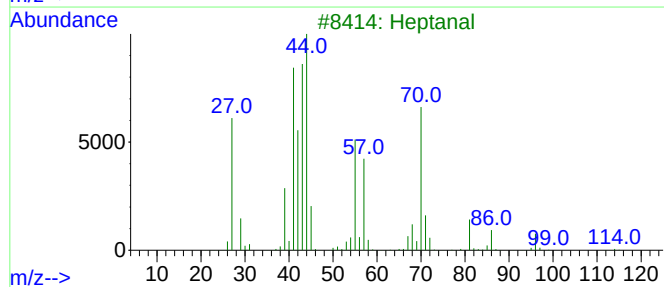
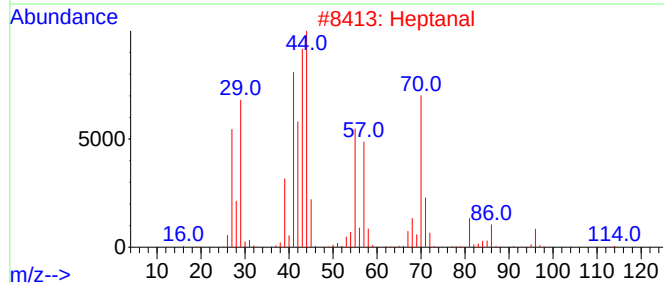
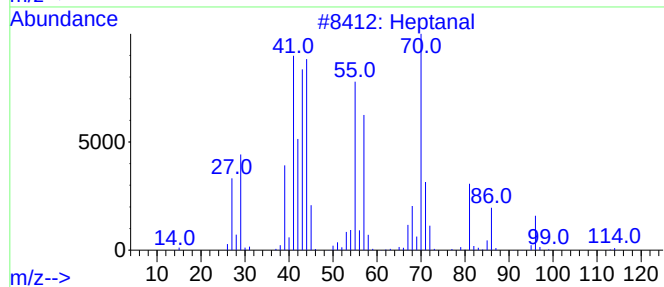
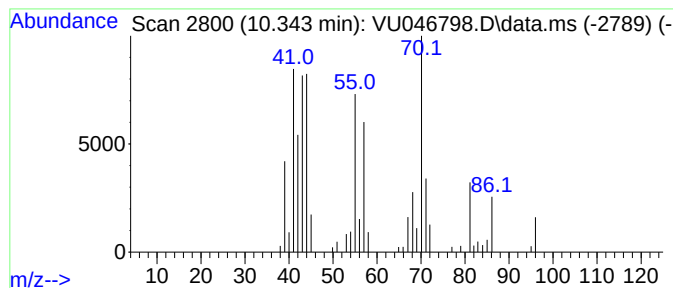
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Heptanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.343	0.99 ug/L	68411	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	86
2	Heptanal			114	C7H14O	000111-71-7	64
3	Heptanal			114	C7H14O	000111-71-7	64
4	Heptanal			114	C7H14O	000111-71-7	64
5	Heptanal			114	C7H14O	000111-71-7	59



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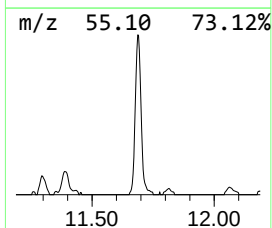
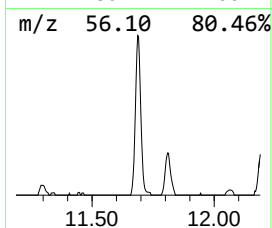
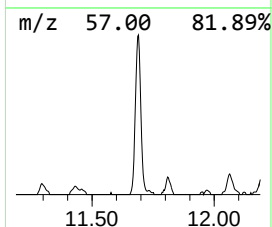
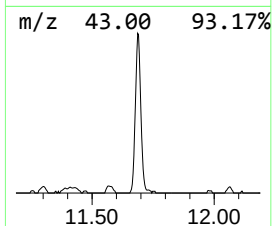
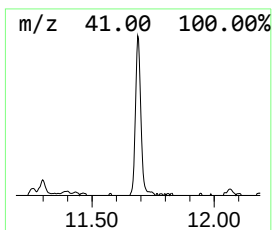
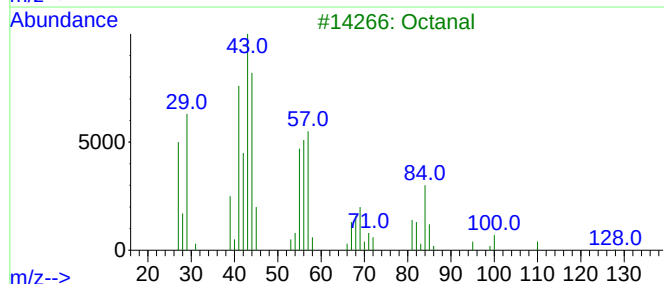
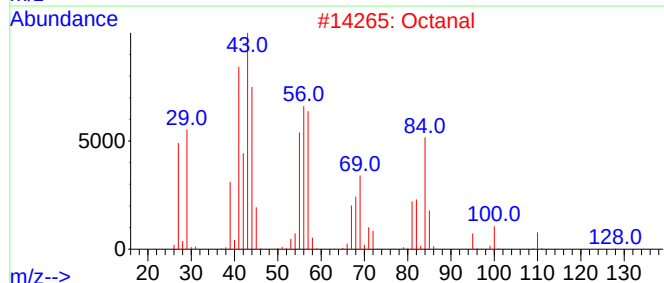
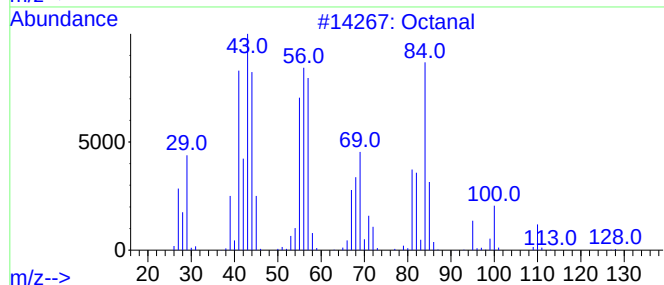
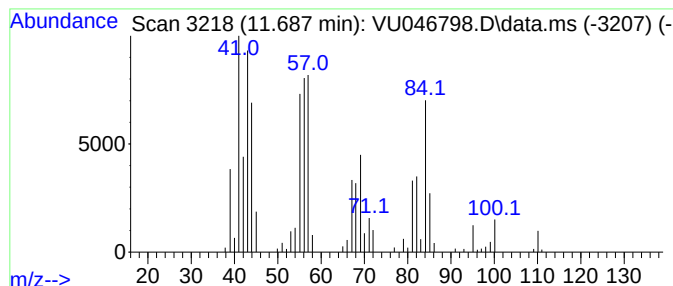
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	2.01 ug/L	160971	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	90
3	Octanal			128	C8H16O	000124-13-0	90
4	Octanal			128	C8H16O	000124-13-0	87
5	Octanal			128	C8H16O	000124-13-0	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046798.D
Acq On : 19 Jan 2022 15:00
Operator : SY/MD
Sample : N1194-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX2

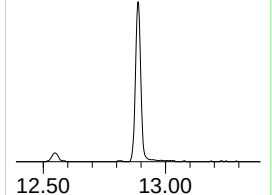
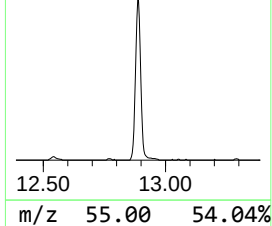
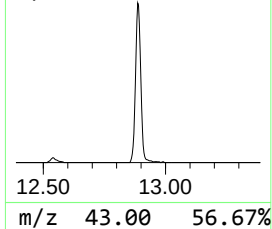
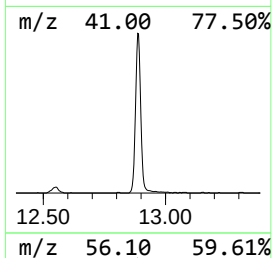
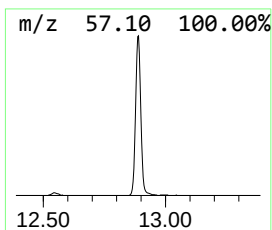
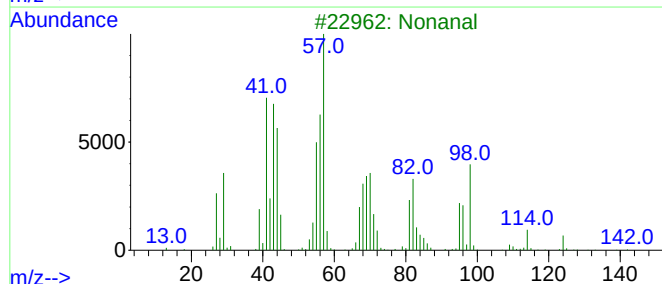
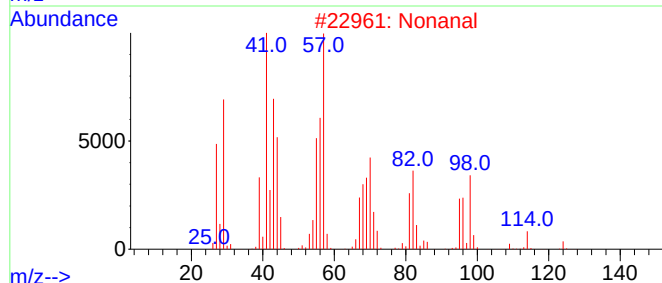
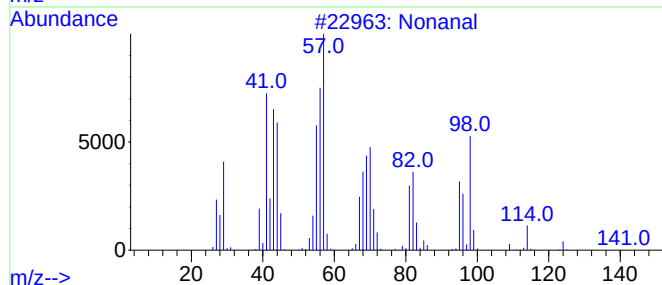
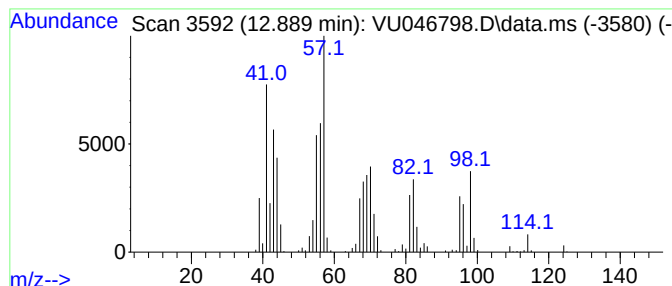
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.889	6.06 ug/L	484795	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Nonanal	142	C9H18O	000124-19-6	91
3			Nonanal	142	C9H18O	000124-19-6	86
4			Nonanal	142	C9H18O	000124-19-6	83
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046798.D
Acq On : 19 Jan 2022 15:00
Operator : SY/MD
Sample : N1194-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

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	1.3	ug/L	63446	1	6.250	254710	5.0
unknown-01	1.475	1.2	ug/L	60062	1	6.250	254710	5.0
Pentanal	6.883	0.9	ug/L	43573	1	6.250	254710	5.0
Hexanal	8.787	5.1	ug/L	355509	2	9.420	346423	5.0
Heptanal	10.343	1.0	ug/L	68411	2	9.420	346423	5.0
Octanal	11.687	2.0	ug/L	160971	3	11.812	400141	5.0
Nonanal	12.889	6.1	ug/L	484795	3	11.812	400141	5.0