

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012022\
 Data File : VU046808.D
 Acq On : 20 Jan 2022 14:02
 Operator : SY/MD
 Sample : N1194-01DL 4X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX1DL

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: VU046808.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	37	47	62	rVB2	25031	31406	3.72%	0.656%
2	1.600	71	81	96	rVB	49249	64514	7.64%	1.348%
3	1.919	171	180	197	rBV	37357	51845	6.14%	1.084%
4	2.575	367	384	399	rBV2	91196	175138	20.73%	3.661%
5	3.594	689	701	714	rVB3	6622	13886	1.64%	0.290%
6	3.874	756	788	809	rVB2	44243	110927	13.13%	2.319%
7	4.642	1012	1027	1071	rBV	55825	204351	24.19%	4.271%
8	5.066	1143	1159	1180	rBV	68630	155382	18.40%	3.248%
9	5.321	1225	1238	1250	rBV3	5310	11231	1.33%	0.235%
10	5.729	1344	1365	1385	rBV2	134879	356544	42.21%	7.453%
11	6.250	1514	1527	1543	rBV	101463	190375	22.54%	3.979%
12	6.546	1606	1619	1634	rBV	101111	189314	22.41%	3.957%
13	6.693	1652	1665	1681	rBV	86958	165728	19.62%	3.464%
14	6.883	1713	1724	1742	rBV3	9692	20175	2.39%	0.422%
15	7.568	1925	1937	1952	rBV	42201	73300	8.68%	1.532%
16	7.899	2027	2040	2054	rBV	167668	285849	33.84%	5.975%
17	7.973	2055	2063	2075	rVB	10512	18000	2.13%	0.376%
18	8.131	2102	2112	2119	rBV2	8130	12829	1.52%	0.268%
19	8.182	2119	2128	2142	rVB2	27515	45162	5.35%	0.944%
20	8.555	2232	2244	2254	rBV3	8555	13504	1.60%	0.282%
21	8.635	2257	2269	2304	rBV	268790	480337	56.87%	10.040%
22	8.787	2304	2316	2343	rVB	96636	171643	20.32%	3.588%
23	9.420	2499	2513	2537	rBV	159927	265339	31.41%	5.546%
24	10.346	2791	2801	2814	rBV3	24664	38300	4.53%	0.801%
25	10.758	2918	2929	2946	rVB2	81084	128596	15.22%	2.688%
26	11.690	3208	3219	3233	rBV2	62380	95686	11.33%	2.000%
27	11.812	3245	3257	3275	rBV	188471	297137	35.18%	6.211%
28	12.195	3362	3376	3389	rBV	169841	272974	32.32%	5.706%
29	12.889	3579	3592	3618	rBV	580205	844696	100.00%	17.656%

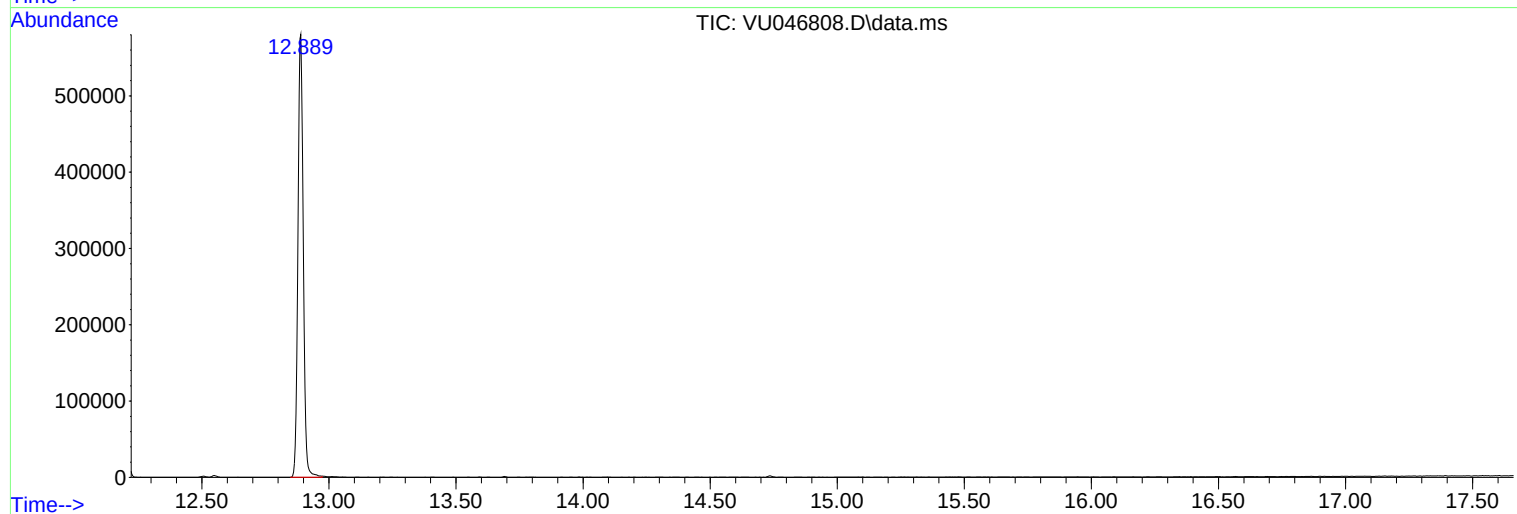
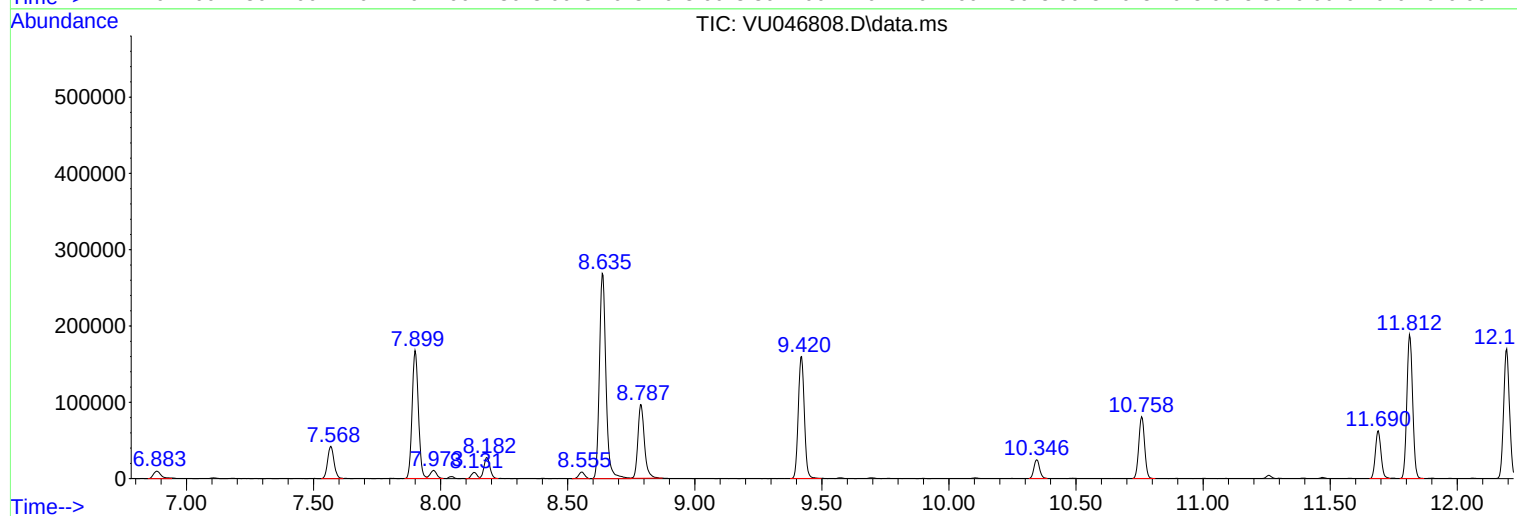
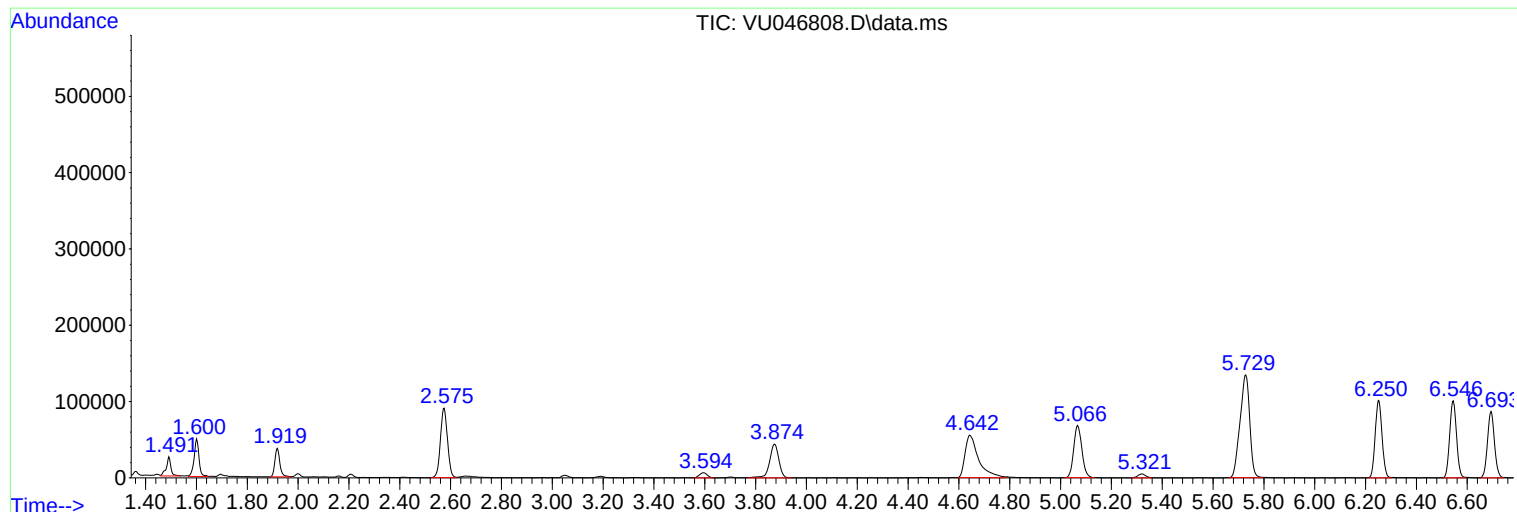
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BFXX1DL

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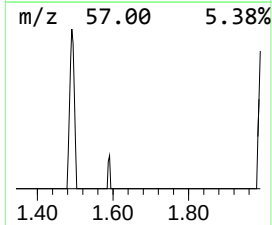
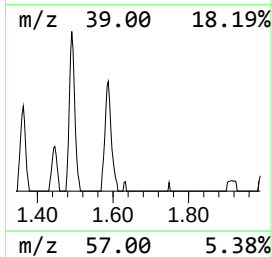
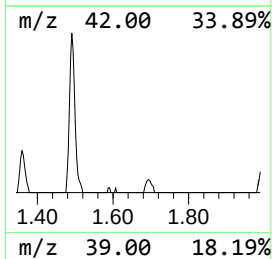
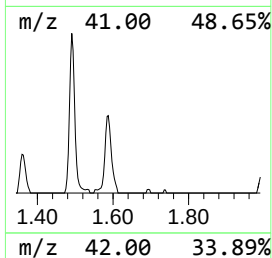
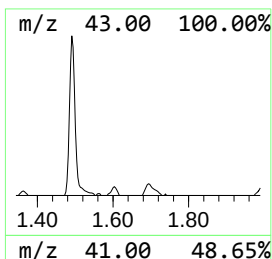
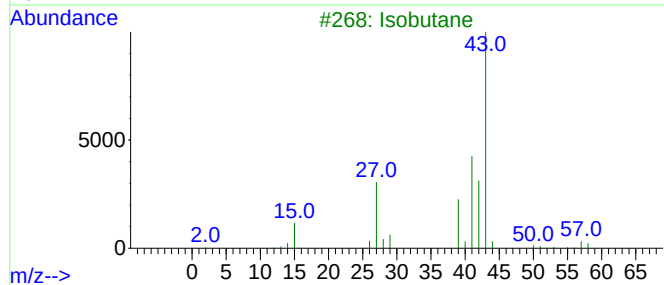
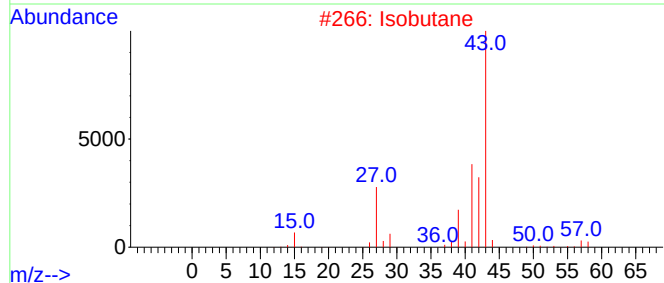
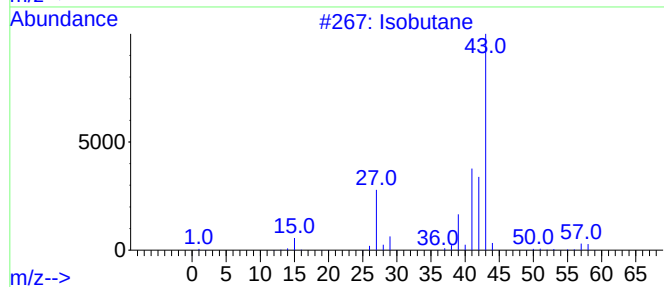
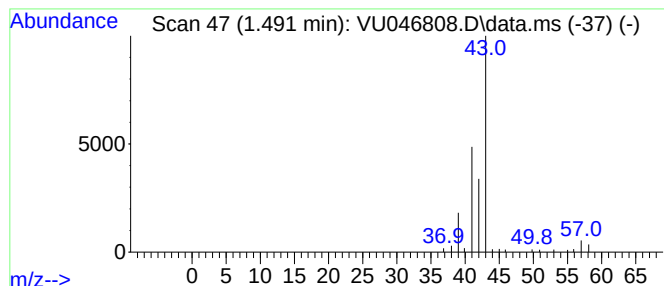
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	0.82 ug/L	31406	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	72
2		Isobutane	58	C4H10	000075-28-5	64
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	50
5		Isobutane	58	C4H10	000075-28-5	45



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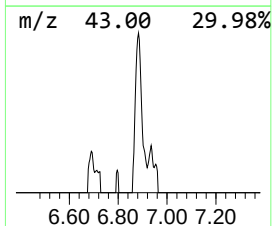
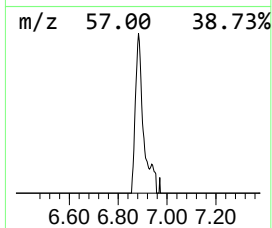
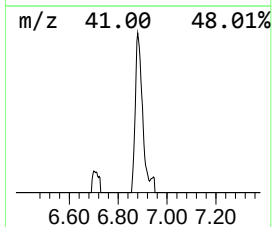
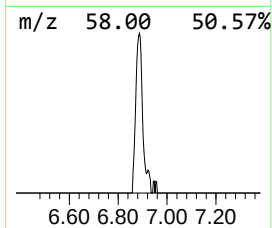
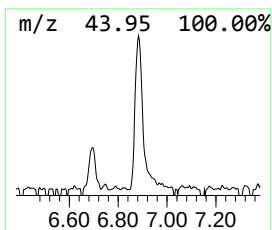
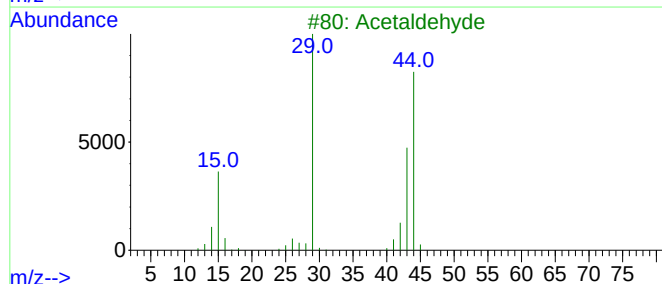
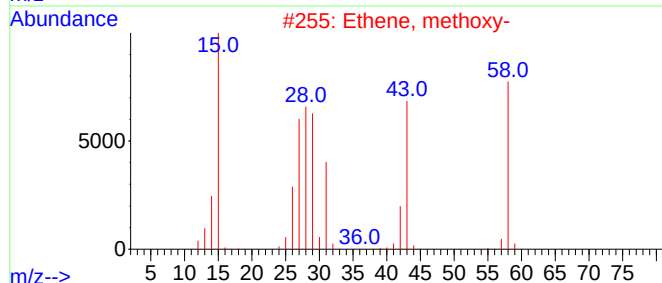
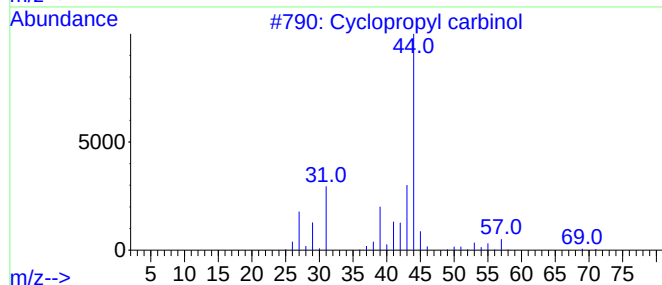
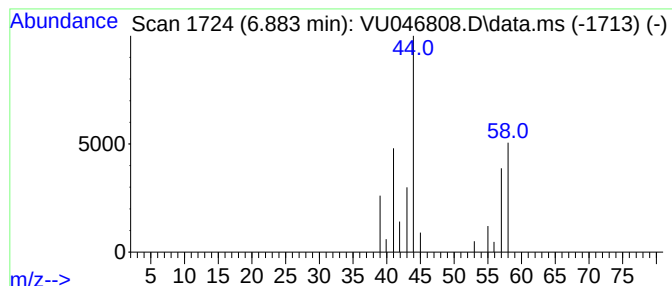
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	0.53 ug/L	20175	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropyl carbinol	72	C4H8O	002516-33-8	9
2			Ethene, methoxy-	58	C3H6O	000107-25-5	5
3			Acetaldehyde	44	C2H4O	000075-07-0	4
4			Acetaldehyde	44	C2H4O	000075-07-0	4
5			Propane	44	C3H8	000074-98-6	4



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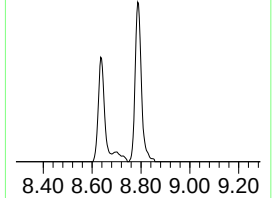
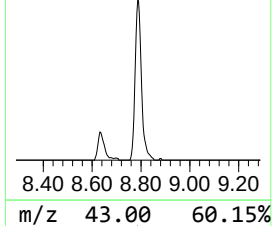
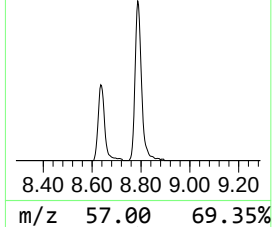
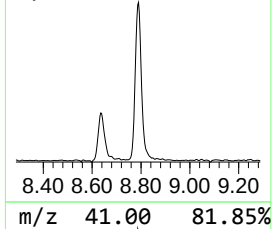
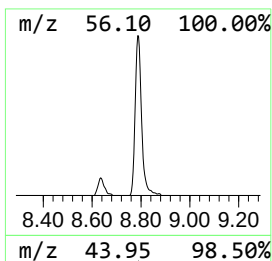
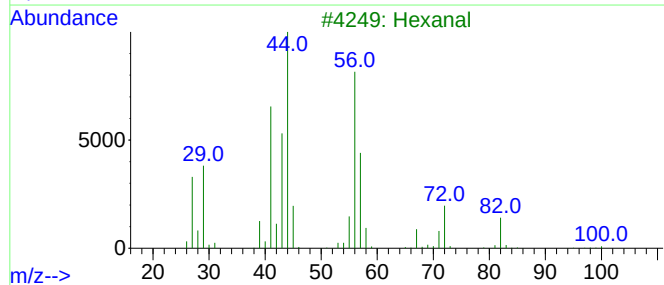
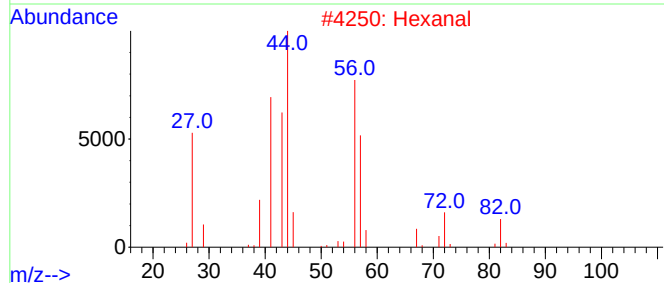
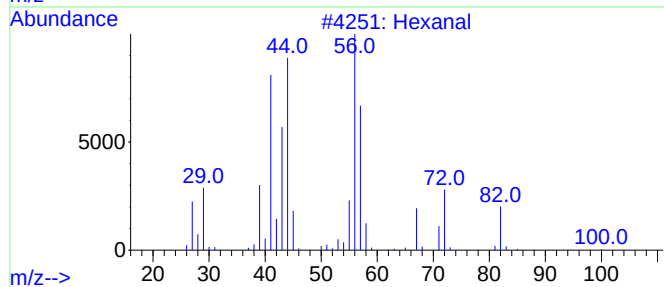
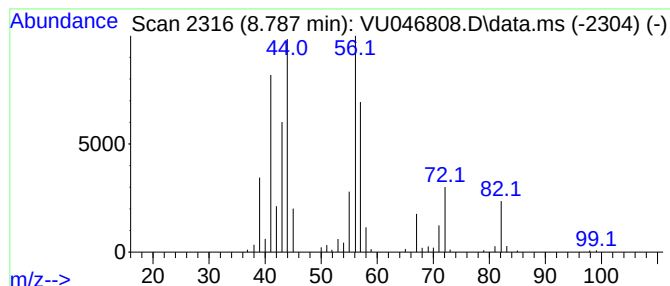
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	3.23 ug/L	171643	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	86
3	Hexanal			100	C6H12O	000066-25-1	83
4	Hexanal			100	C6H12O	000066-25-1	83
5	Hexanal			100	C6H12O	000066-25-1	72



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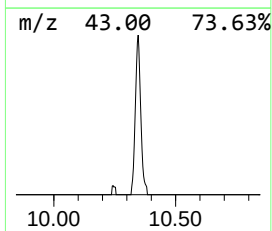
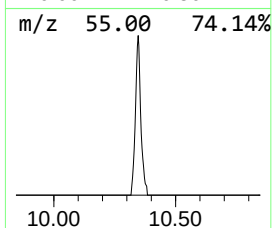
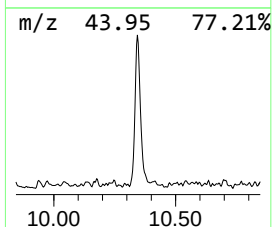
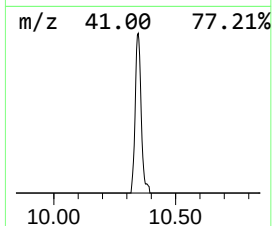
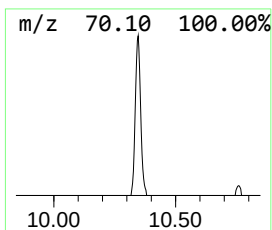
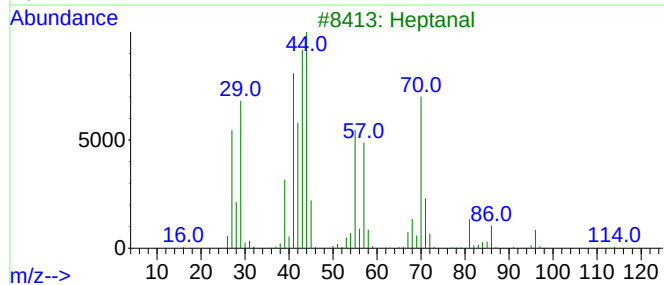
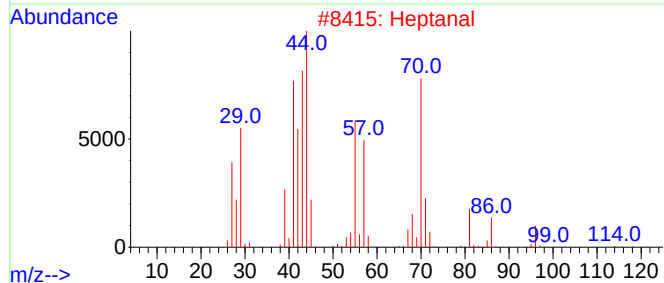
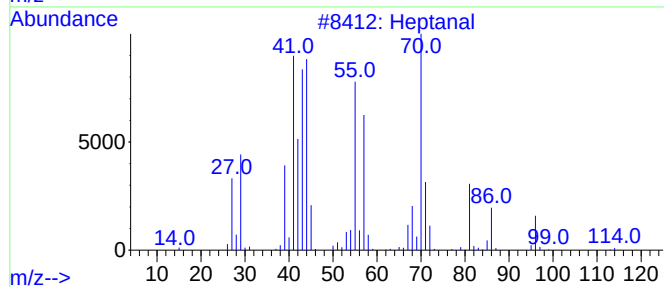
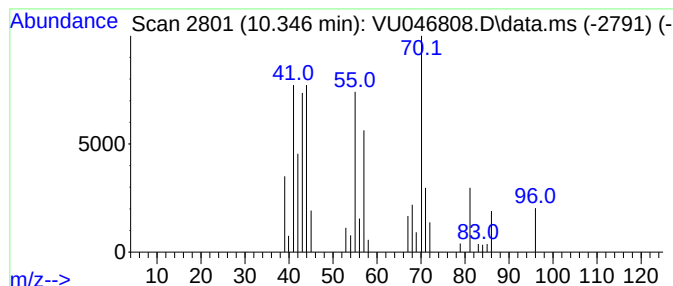
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.346	0.72 ug/L	38300	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	90
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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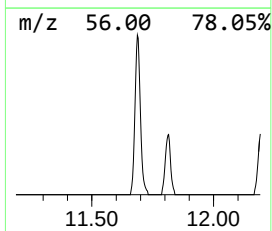
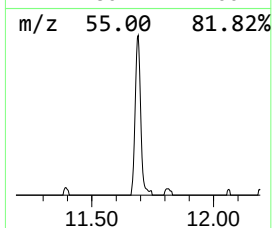
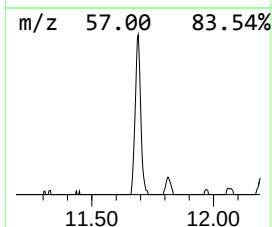
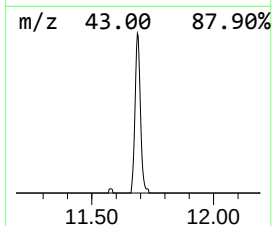
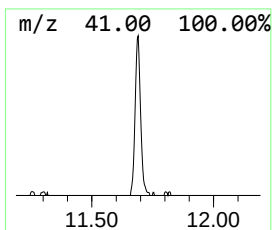
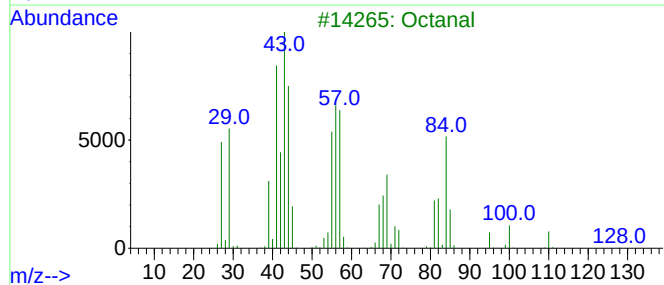
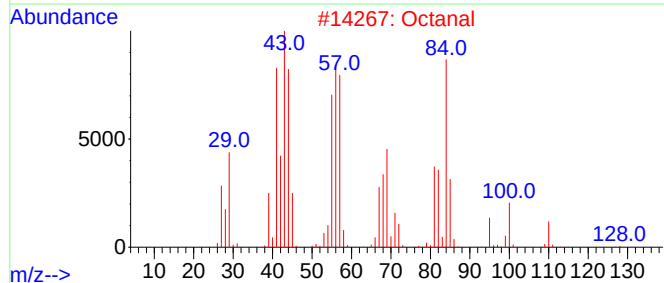
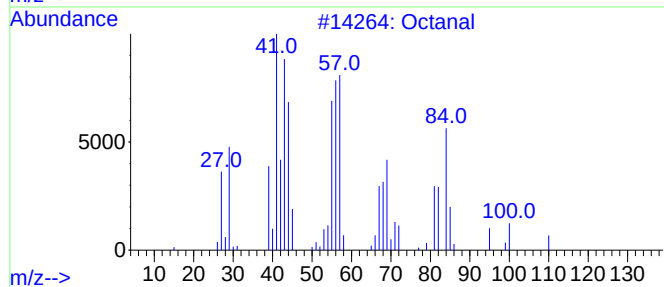
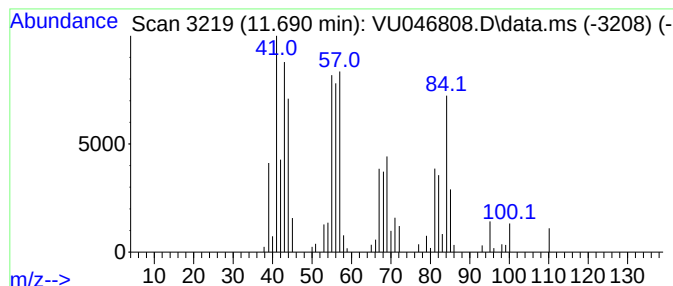
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.690	1.61 ug/L	95686	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	78
4	Cyclopentanol, 2-methyl-, trans-			100	C6H12O	025144-04-1	38
5	Cyclopentanone			84	C5H8O	000120-92-3	38



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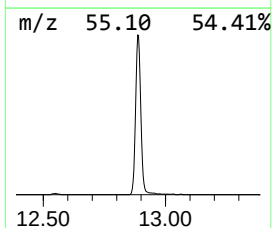
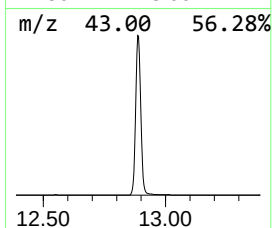
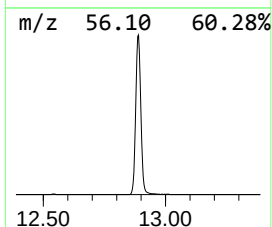
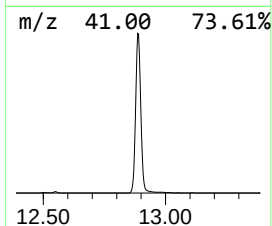
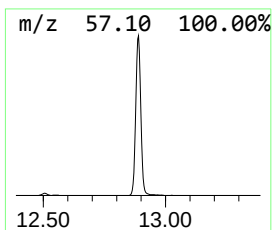
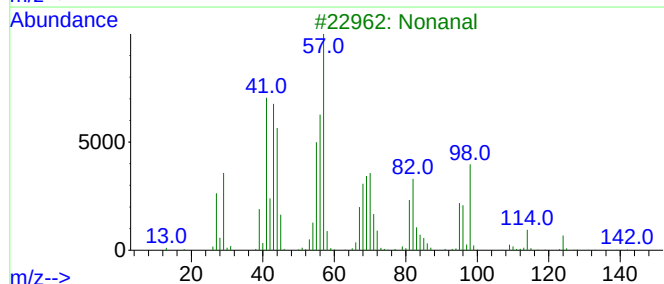
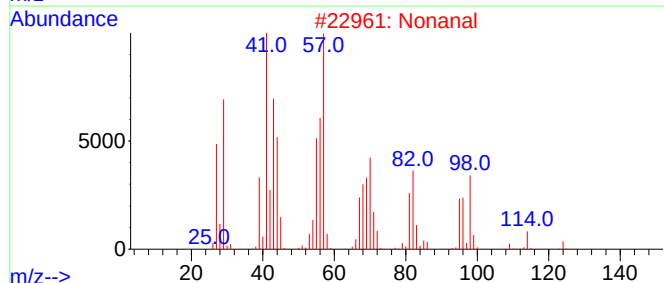
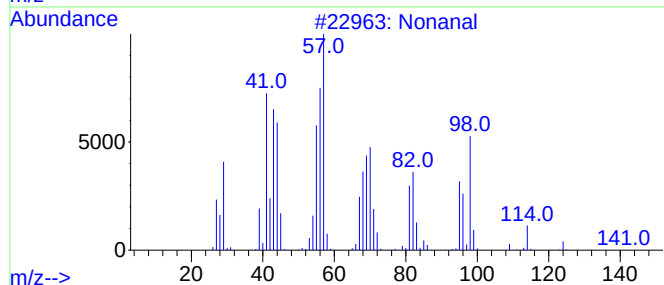
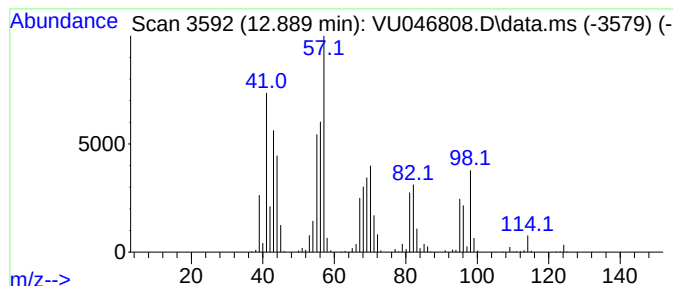
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.889	14.21 ug/L	844696	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	91
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\VU012022\
Data File : VU046808.D
Acq On : 20 Jan 2022 14:02
Operator : SY/MD
Sample : N1194-01DL 4X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1DL

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...	1.491	0.8	ug/L	31406	1	6.253	190375	5.0
unknown-01	6.883	0.5	ug/L	20175	1	6.253	190375	5.0
Hexanal	8.787	3.2	ug/L	171643	2	9.420	265339	5.0
Heptanal	10.346	0.7	ug/L	38300	2	9.420	265339	5.0
Octanal	11.690	1.6	ug/L	95686	3	11.812	297137	5.0
Nonanal	12.889	14.2	ug/L	844696	3	11.812	297137	5.0