

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012622\
 Data File : VU046842.D
 Acq On : 26 Jan 2022 13:48
 Operator : SY/MD
 Sample : N1260-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFX6

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: VU046842.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	75	82	98	rVB	55782	65014	5.94%	1.201%
2	1.919	172	180	196	rVB	41811	55513	5.08%	1.026%
3	2.572	365	383	403	rBV2	99207	197081	18.02%	3.641%
4	3.874	773	788	805	rVB	15735	37514	3.43%	0.693%
5	4.652	1015	1030	1032	rBV2	41483	70044	6.40%	1.294%
6	5.070	1143	1160	1184	rBV	76563	179294	16.39%	3.313%
7	5.729	1345	1365	1388	rBV2	148389	386529	35.34%	7.142%
8	6.253	1513	1528	1546	rBV	118326	221811	20.28%	4.098%
9	6.694	1651	1665	1686	rBV2	91352	181502	16.60%	3.353%
10	6.883	1713	1724	1744	rBV2	37292	76474	6.99%	1.413%
11	7.568	1926	1937	1957	rBV2	42351	74413	6.80%	1.375%
12	7.899	2028	2040	2056	rBV	168135	295665	27.03%	5.463%
13	8.182	2118	2128	2142	rBV	27451	45733	4.18%	0.845%
14	8.636	2257	2269	2296	rBV	255188	469695	42.95%	8.678%
15	8.787	2303	2316	2361	rVB	604811	1093670	100.00%	20.207%
16	9.420	2500	2513	2531	rBV	184898	309305	28.28%	5.715%
17	10.346	2791	2801	2823	rVB2	46498	80385	7.35%	1.485%
18	10.758	2918	2929	2944	rVB	82957	132812	12.14%	2.454%
19	11.295	3087	3096	3105	rVB2	17174	25762	2.36%	0.476%
20	11.690	3207	3219	3245	rBV2	119932	195336	17.86%	3.609%
21	11.812	3245	3257	3274	rVB	220904	347613	31.78%	6.423%
22	12.195	3363	3376	3394	rVB	172490	283721	25.94%	5.242%
23	12.545	3473	3485	3499	rBV4	32069	55406	5.07%	1.024%
24	12.889	3580	3592	3617	rBV	215100	326541	29.86%	6.033%
25	13.684	3828	3839	3849	rVB4	9050	12606	1.15%	0.233%
26	14.732	4154	4165	4180	rBV2	102521	157218	14.38%	2.905%
27	15.706	4459	4468	4479	rBV4	23926	35762	3.27%	0.661%

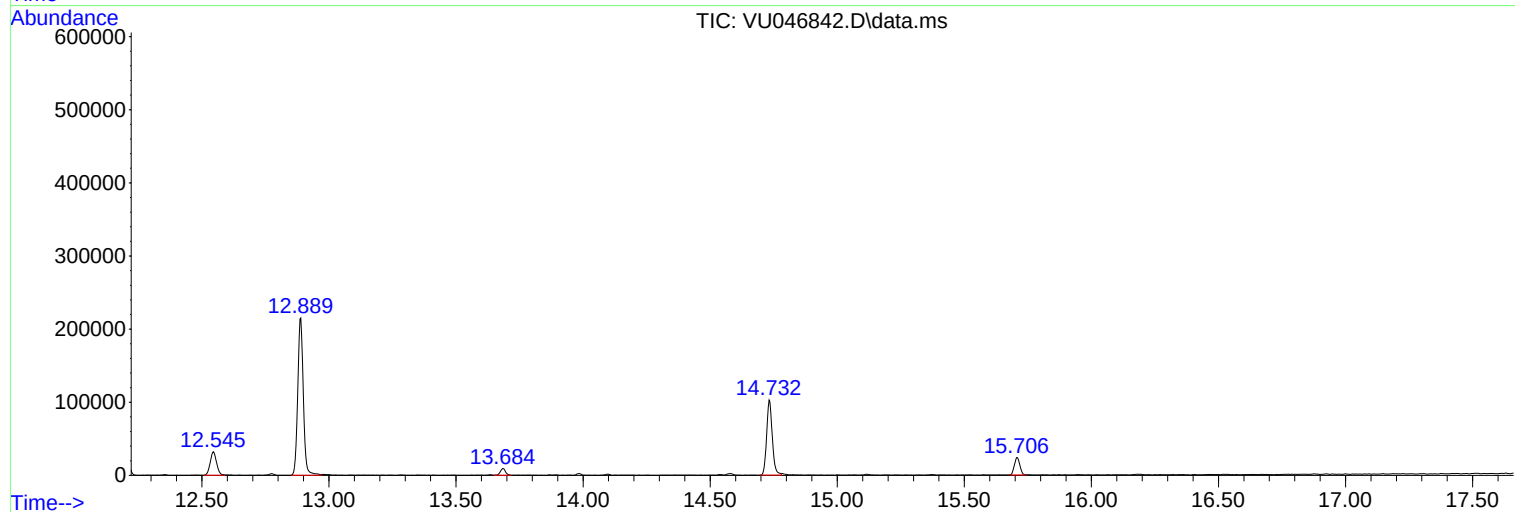
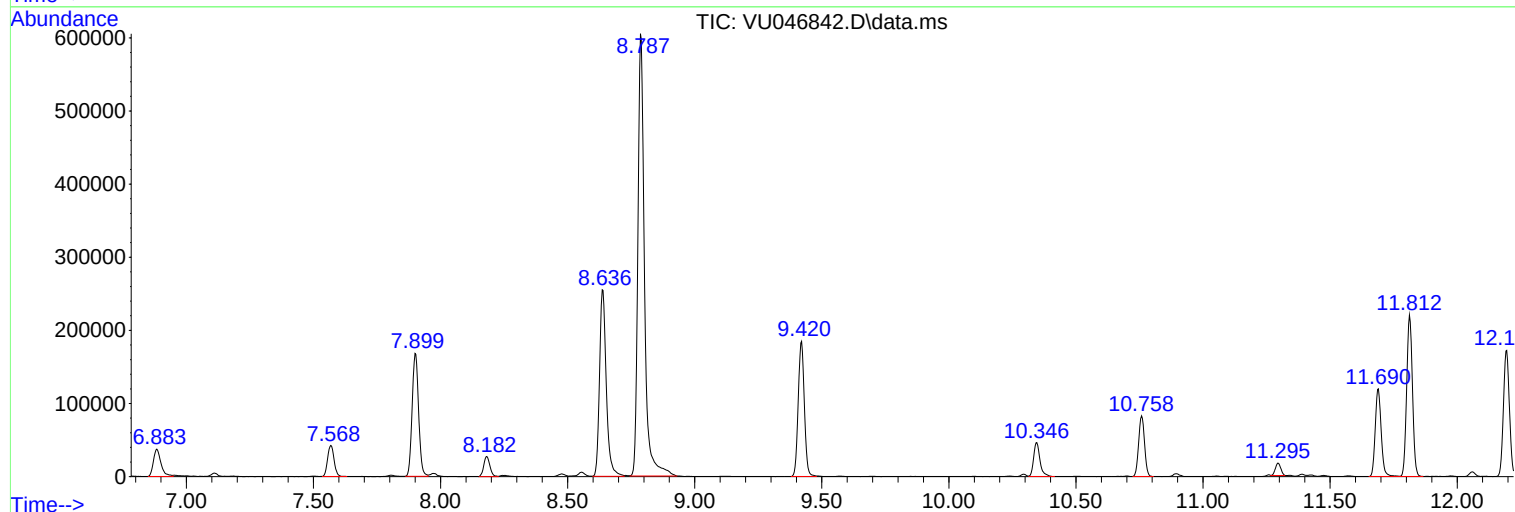
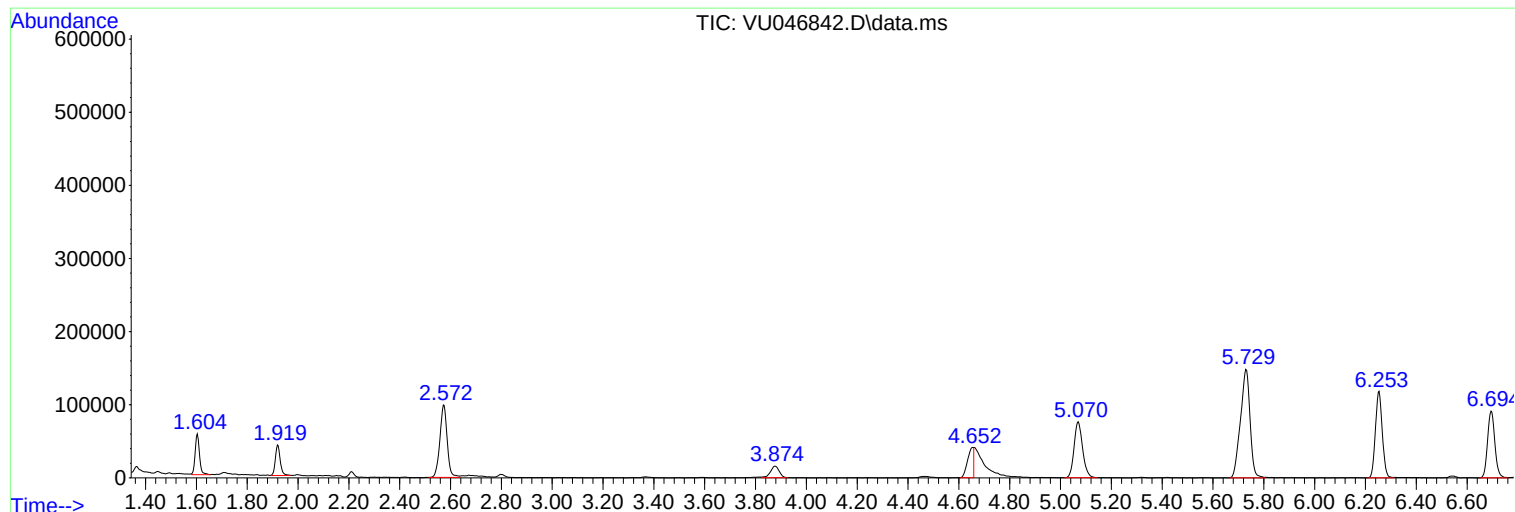
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MSVOA_U
ClientSampleId :
BFX6

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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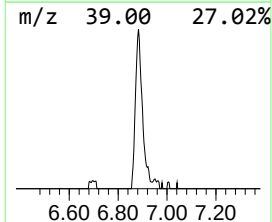
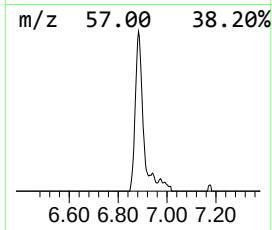
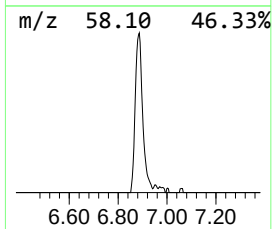
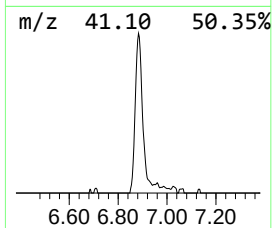
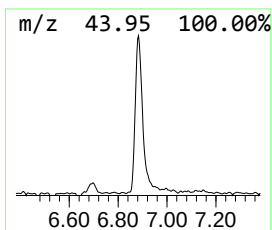
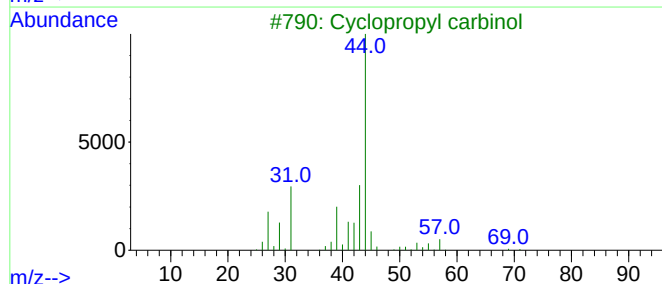
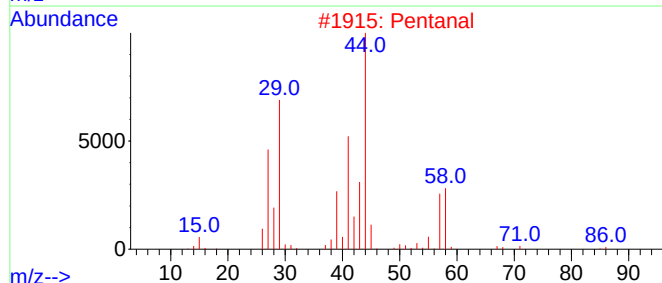
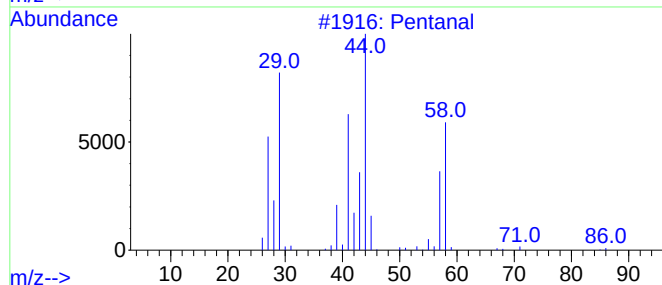
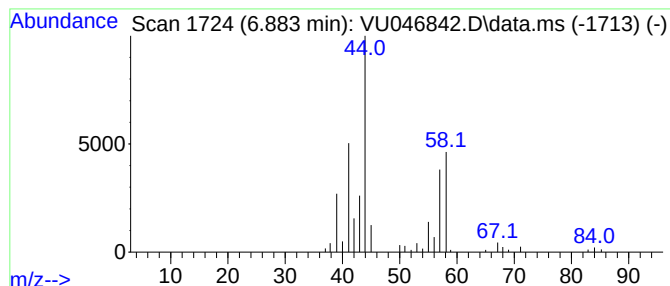
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Pentanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	1.72 ug/L	76474	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	78
2	Pentanal			86	C5H10O	000110-62-3	59
3	Cyclopropyl carbinol			72	C4H8O	002516-33-8	47
4	Pentanal			86	C5H10O	000110-62-3	40
5	Cyclopropyl carbinol			72	C4H8O	002516-33-8	9



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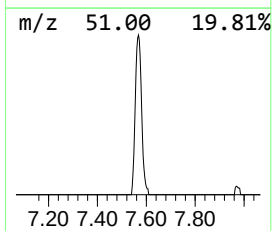
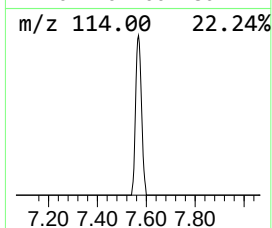
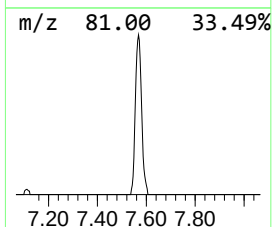
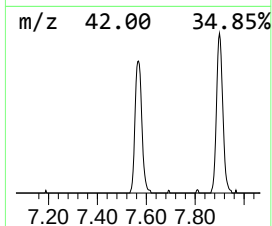
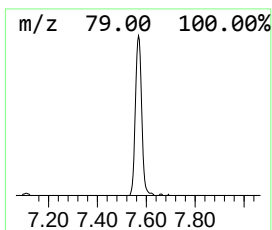
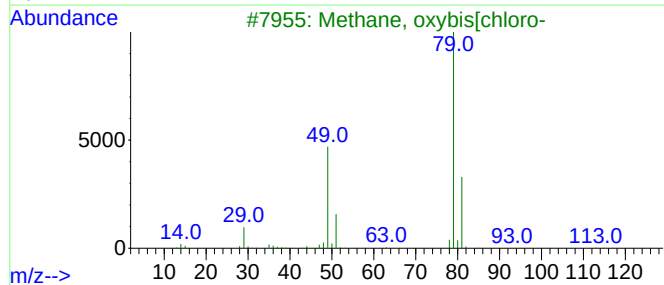
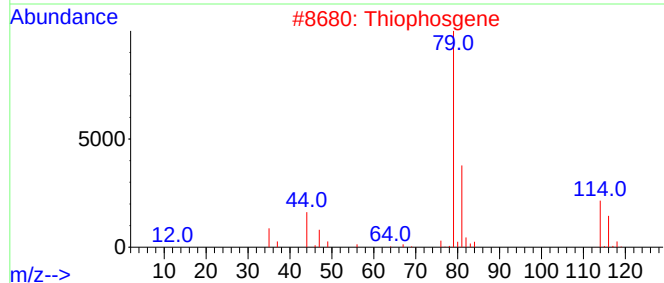
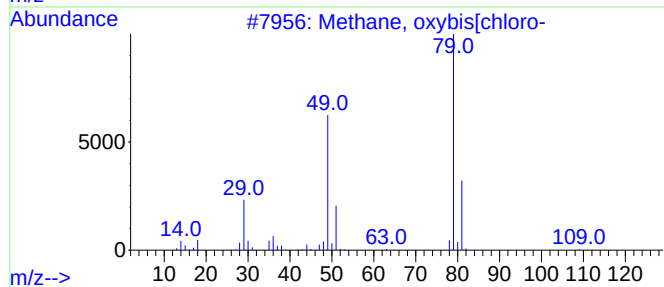
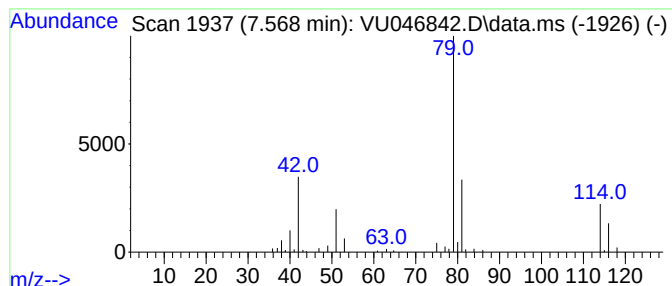
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.568	1.68 ug/L	74413	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	40
2			Thiophosgene	114	CCl2S	000463-71-8	36
3			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	33
4			1,3-Cyclohexadiene	80	C6H8	000592-57-4	28
5			2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	9



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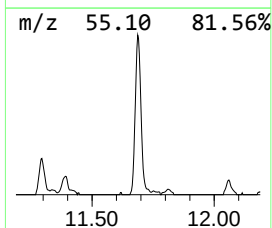
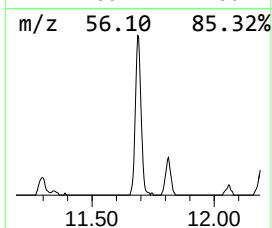
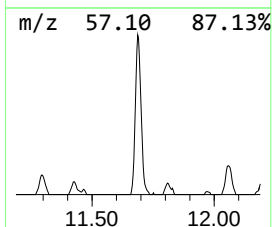
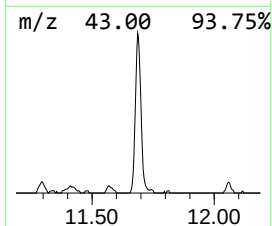
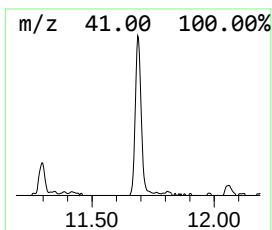
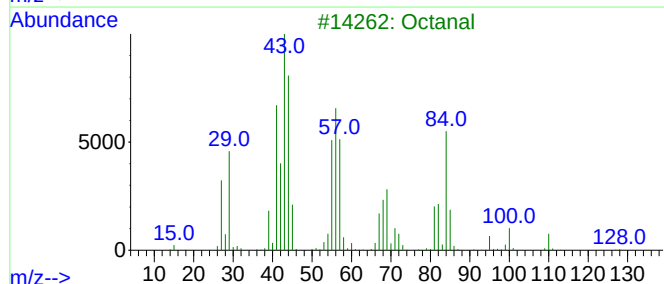
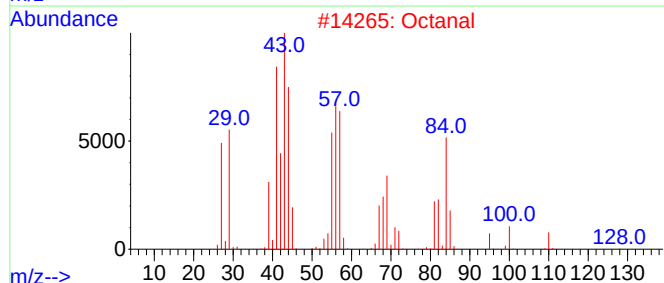
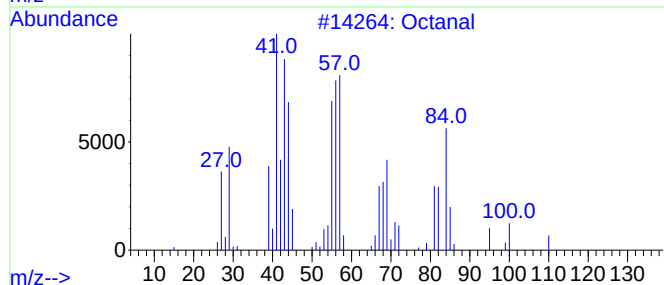
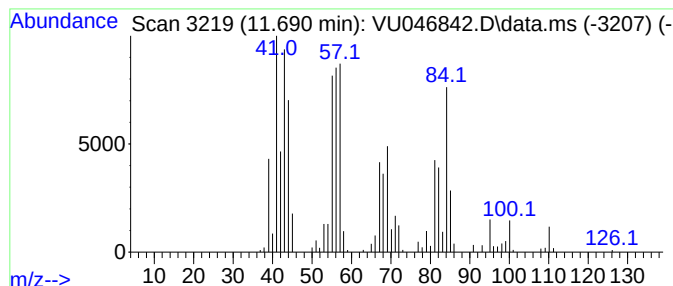
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.690	2.81 ug/L	195336	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	83
3	Octanal			128	C8H16O	000124-13-0	64
4	Octanal			128	C8H16O	000124-13-0	50
5	1-Pentene, 2-methyl-			84	C6H12	000763-29-1	38



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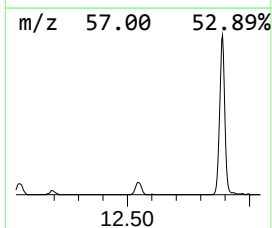
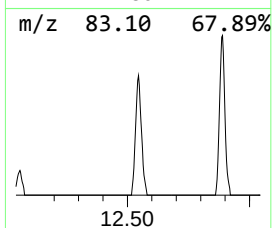
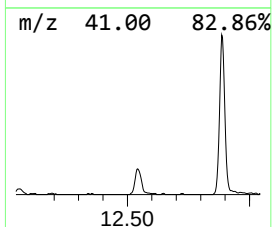
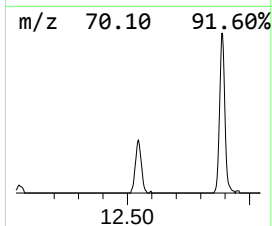
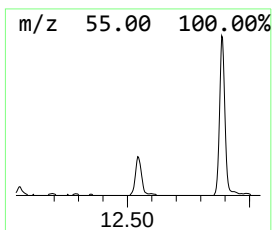
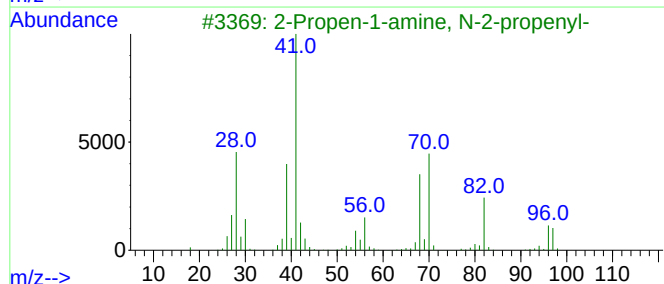
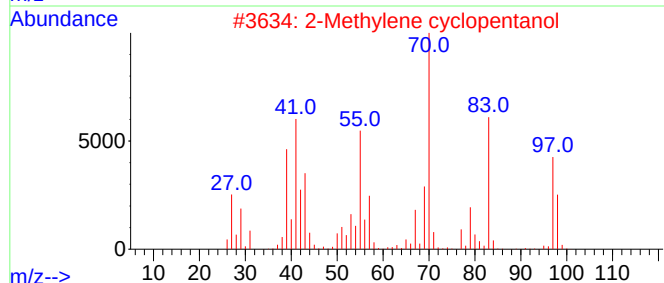
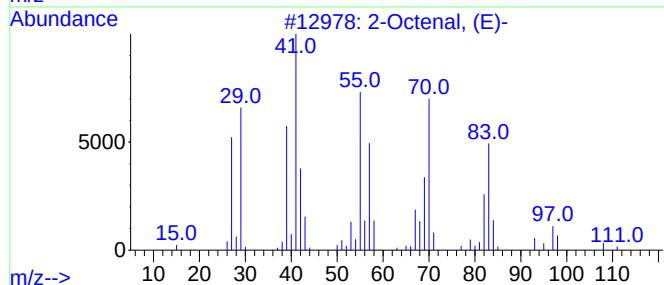
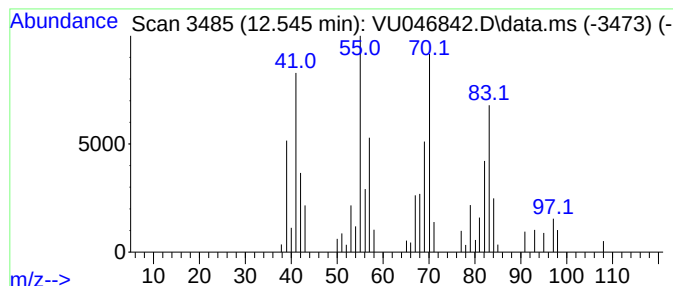
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Octenal, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	0.80 ug/L	55406	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octenal, (E)-	126	C8H14O	002548-87-0	64
2			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	50
3			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	43
4			2-Octenal, (E)-	126	C8H14O	002548-87-0	43
5			2-Octenal, (E)-	126	C8H14O	002548-87-0	43



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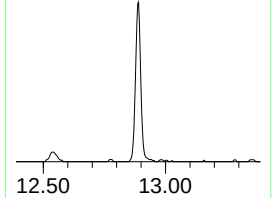
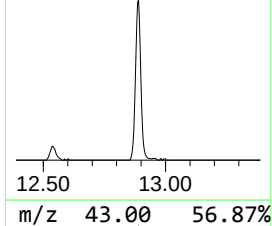
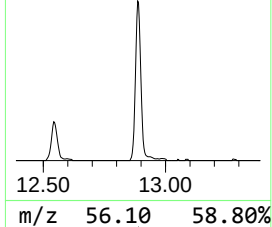
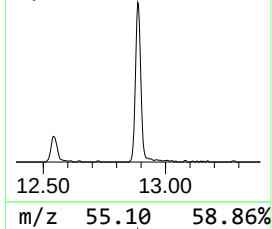
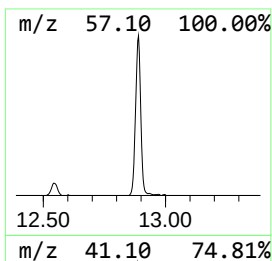
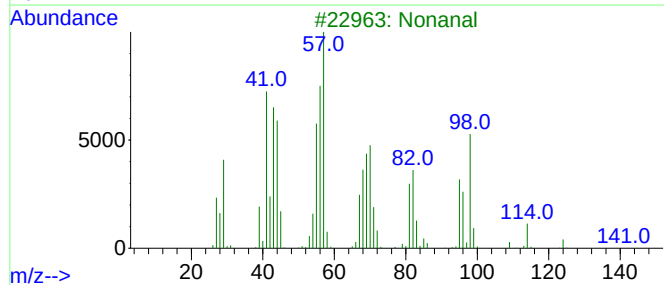
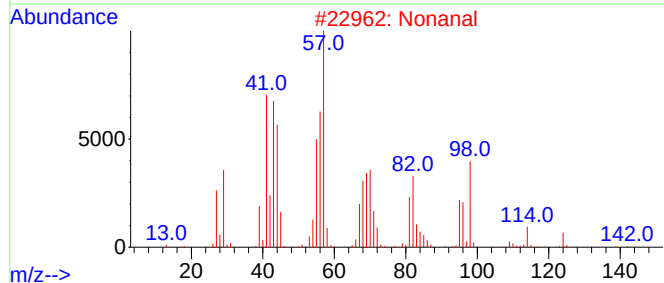
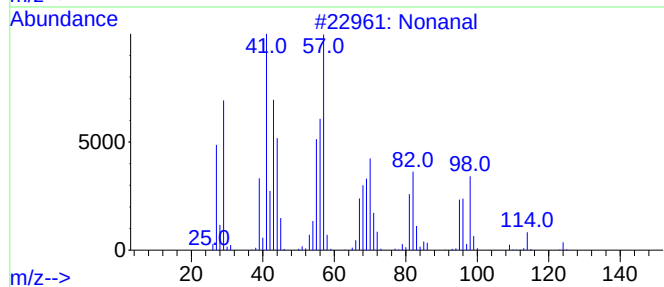
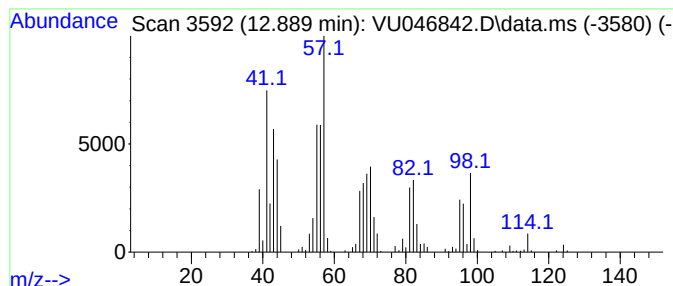
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.889	4.70 ug/L	326541	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			2-Nonen-1-ol, (E)-	142	C9H18O	031502-14-4	35
5			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27



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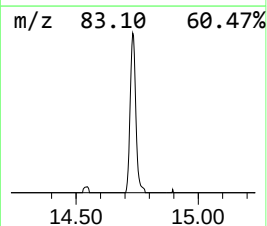
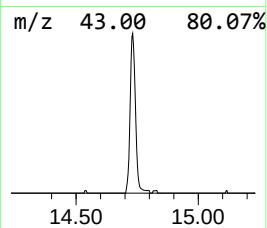
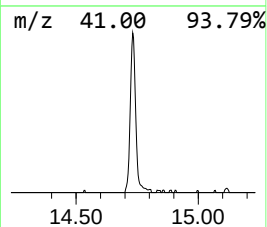
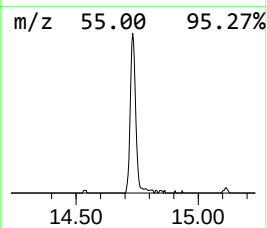
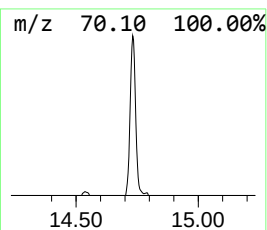
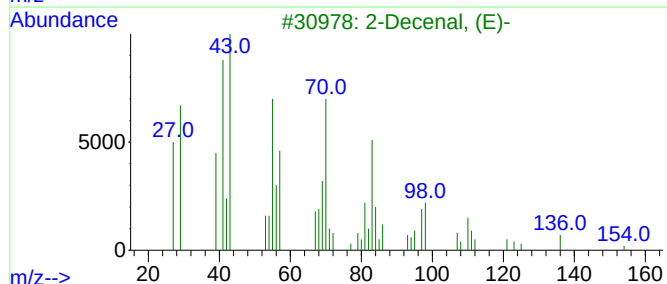
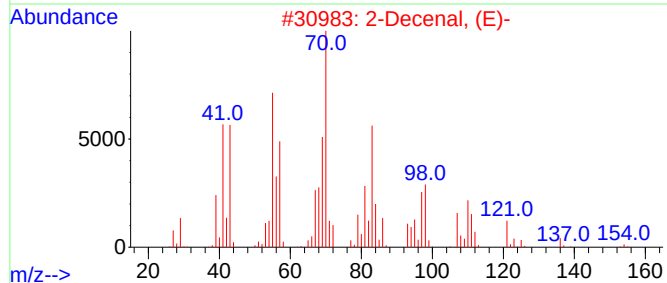
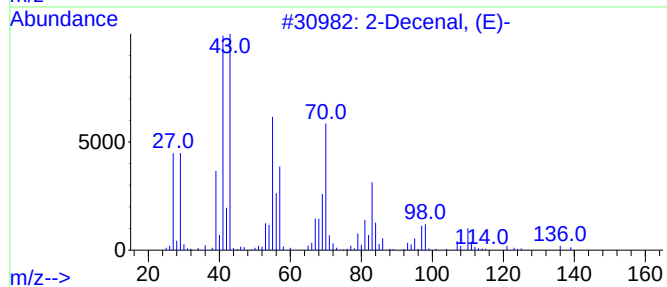
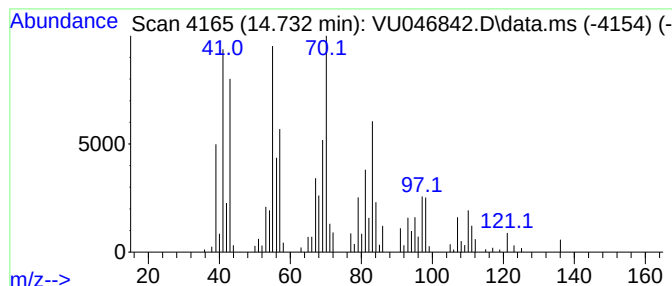
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 2-Decenal, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.732	2.26 ug/L	157218	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenal, (E)-			154	C10H18O	003913-81-3	83
2	2-Decenal, (E)-			154	C10H18O	003913-81-3	74
3	2-Decenal, (E)-			154	C10H18O	003913-81-3	47
4	Cyclopentane, 1,2,3-trimethyl-, ...			112	C8H16	002613-69-6	46
5	Bicyclo[3.1.0]hexan-2-ol			98	C6H10O	1000194-18-6	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012622\
Data File : VU046842.D
Acq On : 26 Jan 2022 13:48
Operator : SY/MD
Sample : N1260-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFX6

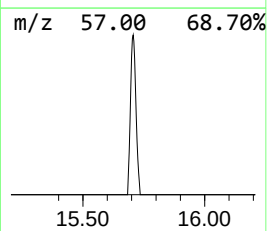
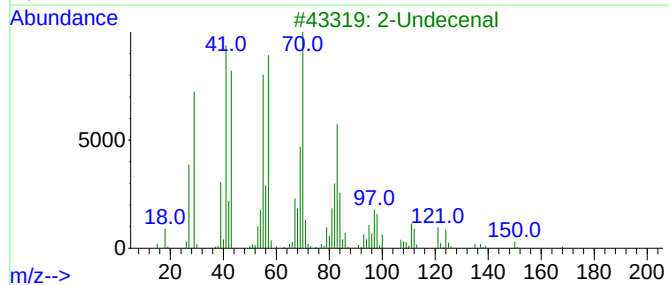
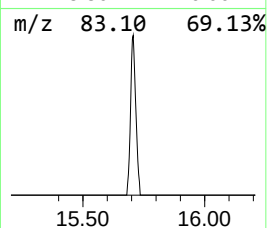
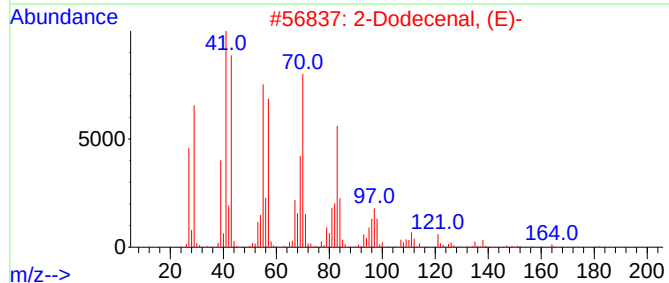
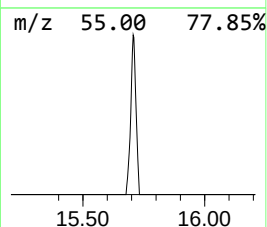
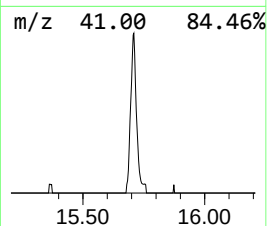
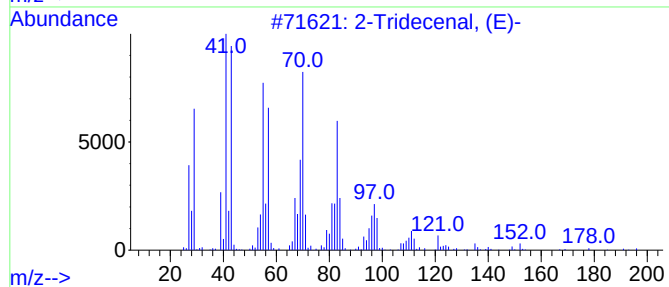
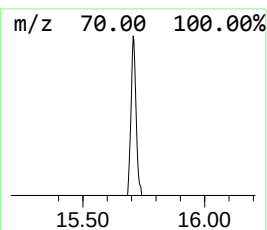
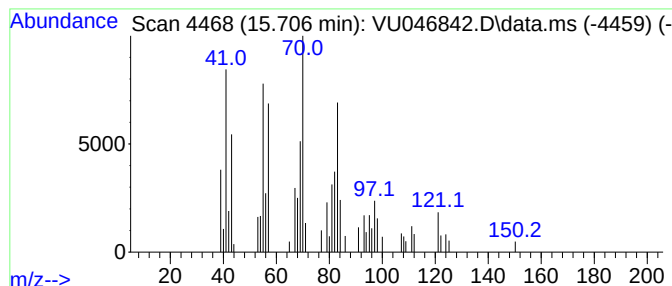
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 2-Tridecenal, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.706	0.51 ug/L	35762	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Tridecenal, (E)-	196	C13H24O	007069-41-2	80
2			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	72
3			2-Undecenal	168	C11H20O	002463-77-6	72
4			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	58
5			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012622\
Data File : VU046842.D
Acq On : 26 Jan 2022 13:48
Operator : SY/MD
Sample : N1260-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX6

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
Pentanal	6.883	1.7	ug/L	76474	1	6.253	221811	5.0
unknown-01	7.568	1.7	ug/L	74413	1	6.253	221811	5.0
Octanal	11.690	2.8	ug/L	195336	3	11.812	347613	5.0
2-Octenal, (E)-	12.545	0.8	ug/L	55406	3	11.812	347613	5.0
Nonanal	12.889	4.7	ug/L	326541	3	11.812	347613	5.0
2-Decenal, (E)-	14.732	2.3	ug/L	157218	3	11.812	347613	5.0
2-Tridecenal, (E)-	15.706	0.5	ug/L	35762	3	11.812	347613	5.0