

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021822\
 Data File : VU047219.D
 Acq On : 17 Feb 2022 21:11
 Operator : SY/MD
 Sample : N1545-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFY03

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\SFAMUTR021622WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU047219.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	27	rVB	323943	318644	2.32%	0.689%
2	1.600	69	81	97	rBV4	278713	477703	3.48%	1.034%
3	2.584	366	387	410	rBV	3554114	5887489	42.90%	12.738%
4	3.877	767	789	812	rBV	256941	614840	4.48%	1.330%
5	4.671	1013	1036	1081	rBV	3910319	8851362	64.50%	19.150%
6	5.070	1145	1160	1184	rVB2	118489	290369	2.12%	0.628%
7	5.321	1216	1238	1260	rVB	476341	1065210	7.76%	2.305%
8	5.729	1344	1365	1378	rBV2	229588	600965	4.38%	1.300%
9	6.253	1514	1528	1549	rVB	179040	342268	2.49%	0.741%
10	6.546	1602	1619	1641	rBV	2252047	4163749	30.34%	9.008%
11	6.694	1652	1665	1682	rVB	143120	279853	2.04%	0.605%
12	6.880	1710	1723	1756	rBV	79124	158527	1.16%	0.343%
13	7.568	1924	1937	1952	rBV	79313	137441	1.00%	0.297%
14	7.902	2024	2041	2055	rBV	288759	524862	3.82%	1.136%
15	8.558	2229	2245	2260	rBV	8077721	13722159	100.00%	29.688%
16	8.636	2260	2269	2303	rVV	391390	799508	5.83%	1.730%
17	8.787	2303	2316	2365	rVB	1391033	2443629	17.81%	5.287%
18	9.420	2499	2513	2534	rBV	264706	471109	3.43%	1.019%
19	10.346	2787	2801	2824	rBV	197738	325842	2.37%	0.705%
20	10.758	2918	2929	2944	rBV	112222	184339	1.34%	0.399%
21	11.687	3206	3218	3232	rBV	499879	732741	5.34%	1.585%
22	11.812	3245	3257	3276	rVB	335747	546142	3.98%	1.182%
23	12.195	3363	3376	3389	rBV	304884	488409	3.56%	1.057%
24	12.545	3472	3485	3501	rBV3	73429	140181	1.02%	0.303%
25	12.886	3577	3591	3615	rBV	1160972	1697064	12.37%	3.672%
26	13.983	3921	3932	3949	rBV	110209	163421	1.19%	0.354%
27	14.735	4154	4166	4198	rBV	410079	627033	4.57%	1.357%
28	15.712	4455	4470	4487	rBV2	91858	166300	1.21%	0.360%

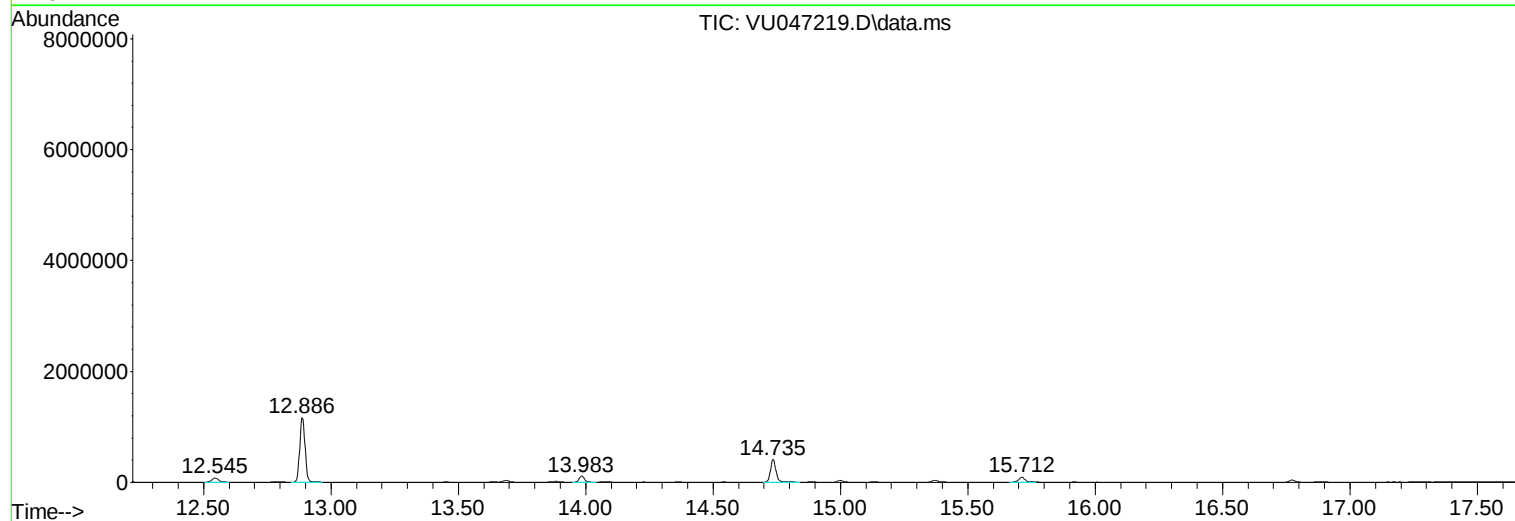
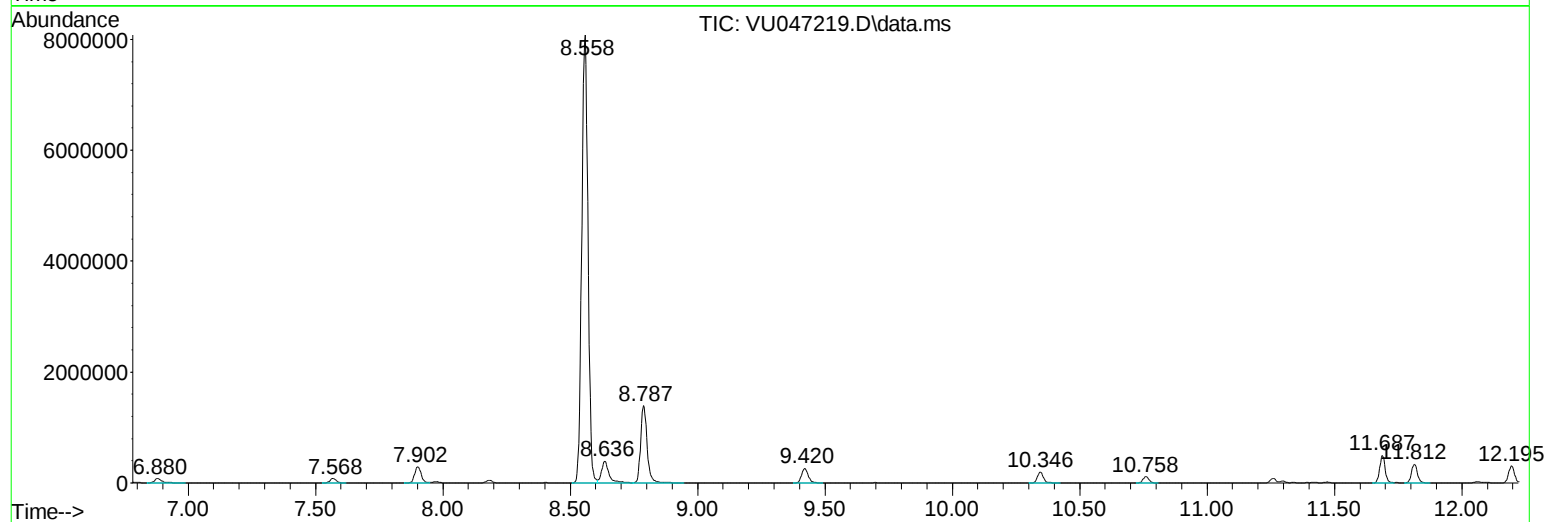
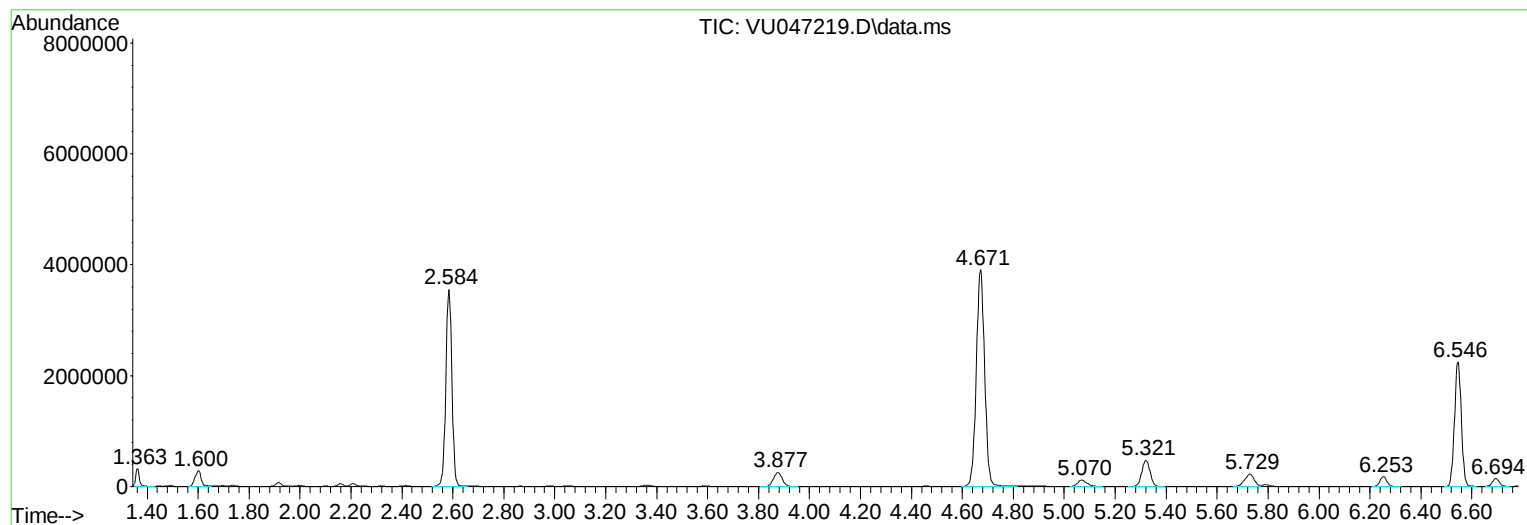
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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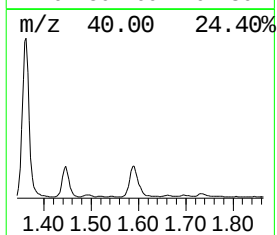
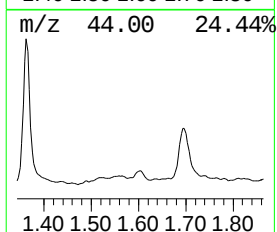
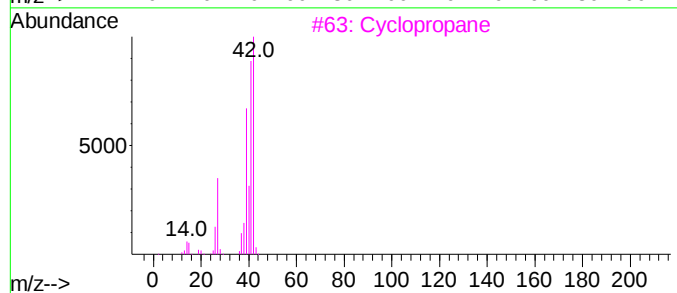
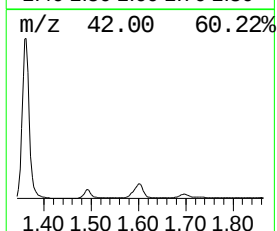
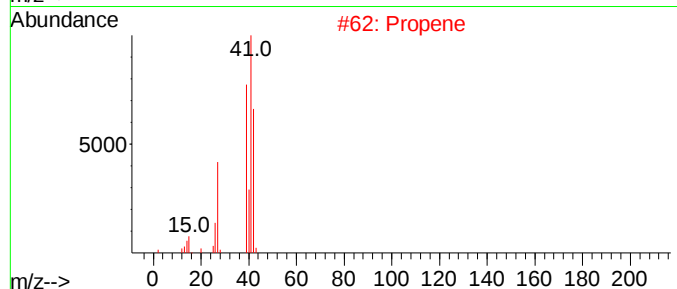
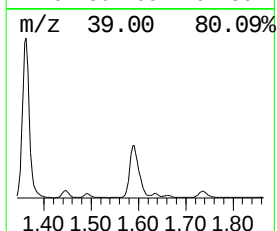
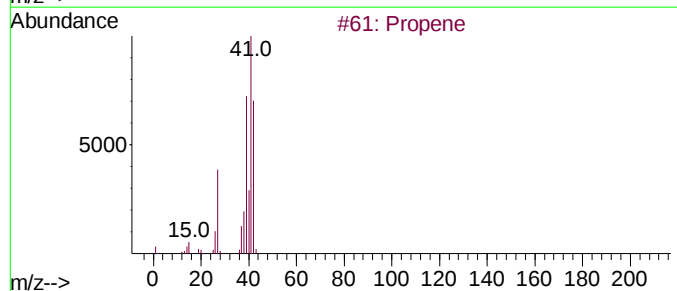
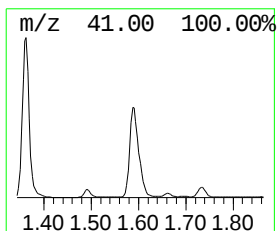
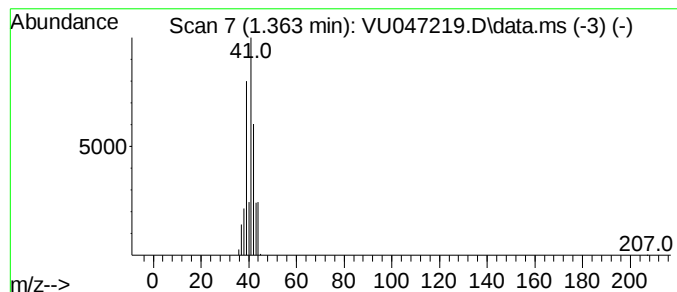
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Quant Title : TRACE VOA SFAM1.0

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	4.65 ug/L	318644	1,4-Difluorobenzene	6.253

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	40
4	Cyclopropane	42	C3H6	000075-19-4	9
5	Cyclopropene	40	C3H4	002781-85-3	9



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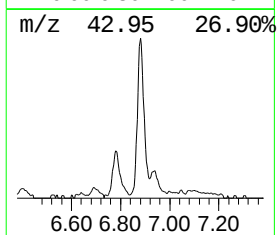
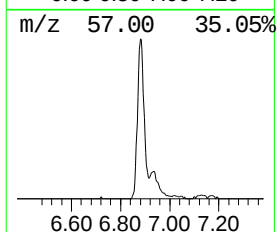
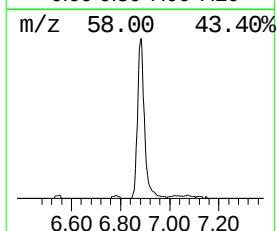
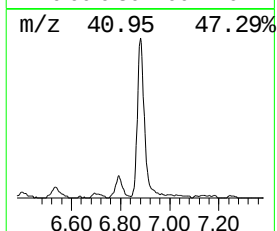
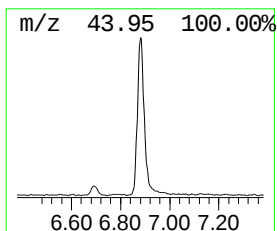
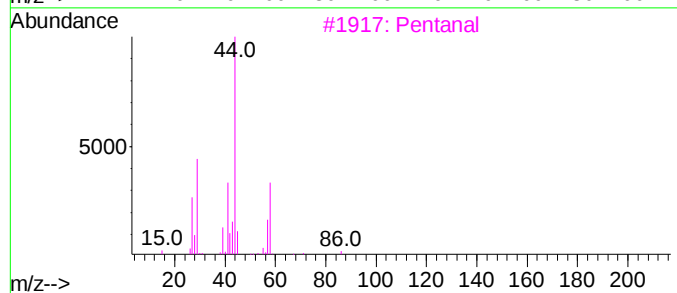
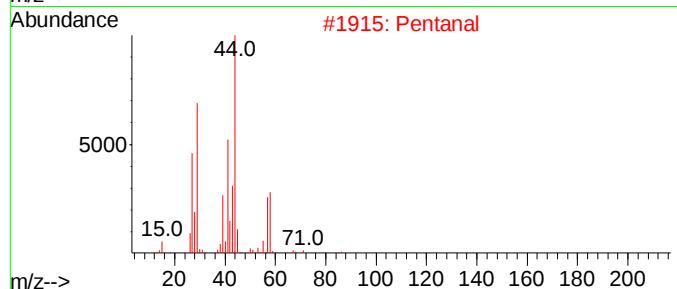
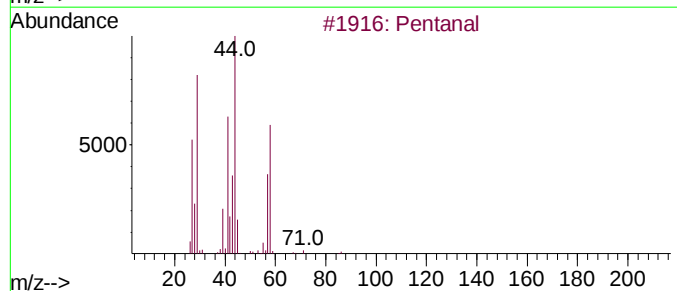
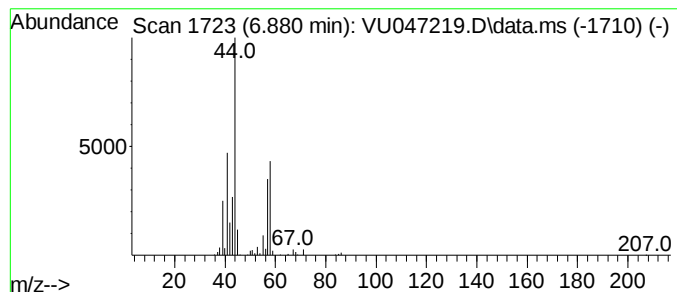
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	2.32 ug/L	158527	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	91
2	Pentanal	86	C5H10O	000110-62-3	86
3	Pentanal	86	C5H10O	000110-62-3	74
4	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
5	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74



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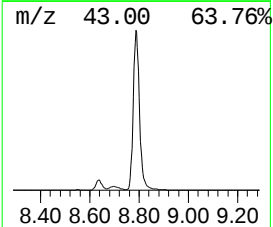
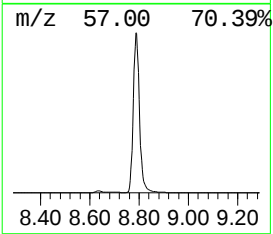
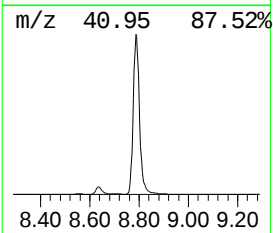
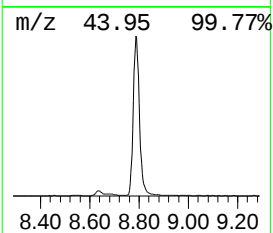
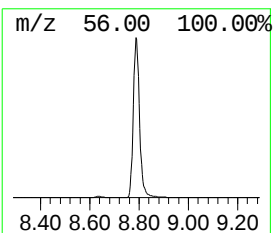
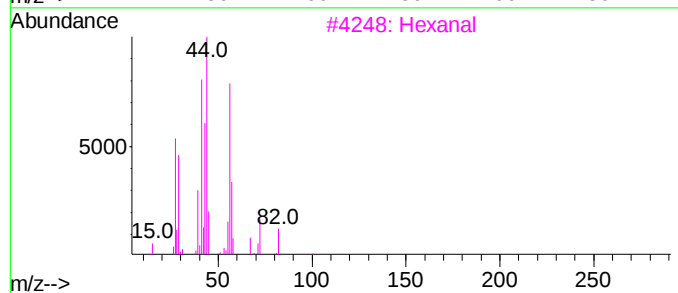
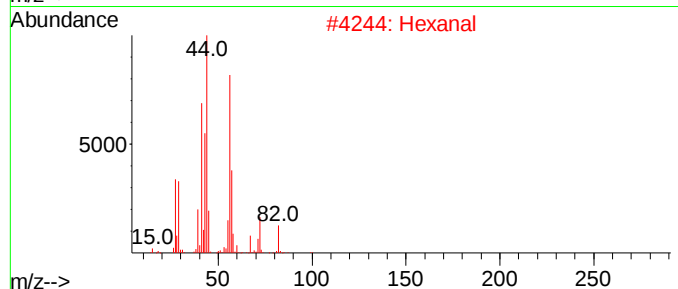
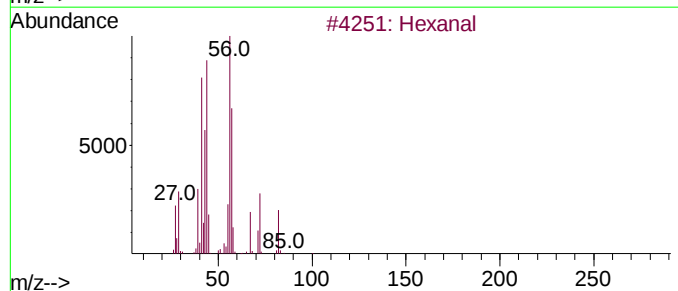
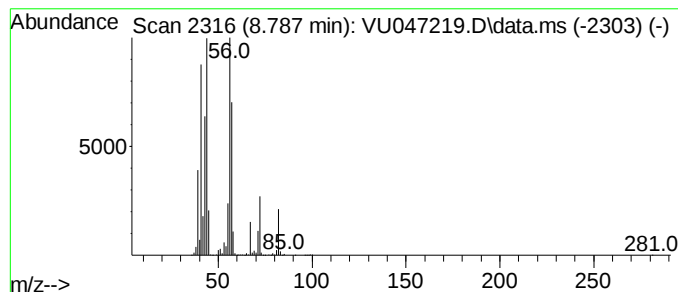
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	25.93 ug/L	2443630	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	87
3	Hexanal			100	C6H12O	000066-25-1	81
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	59



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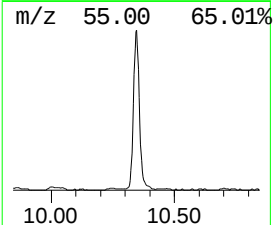
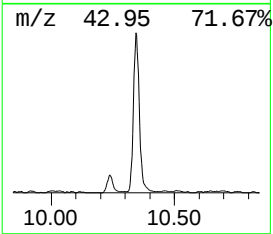
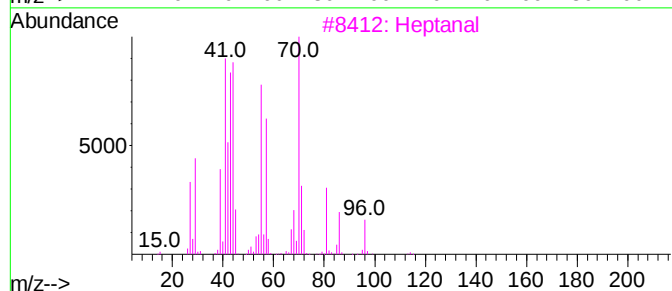
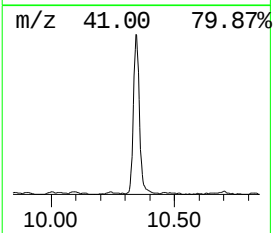
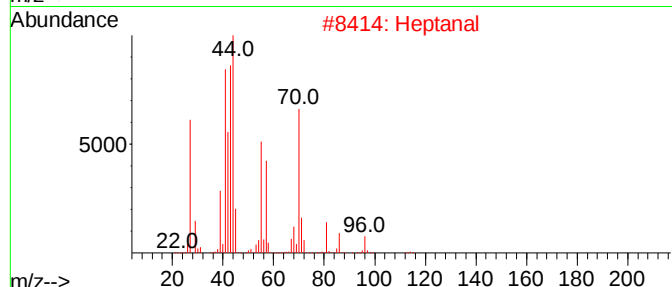
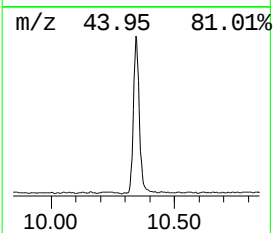
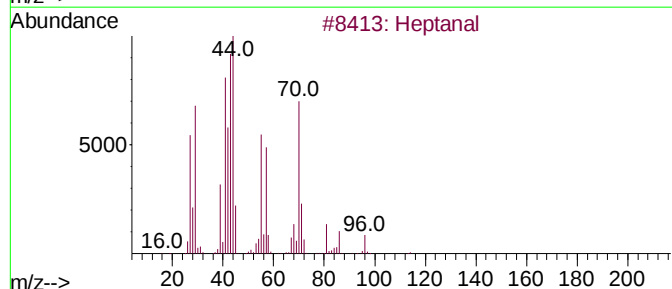
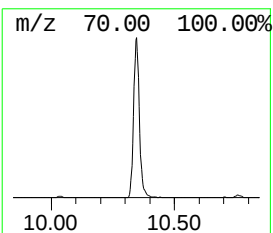
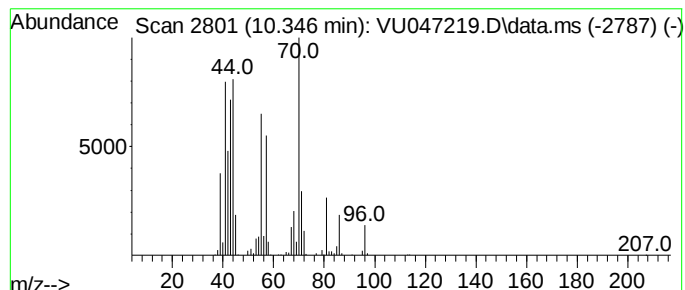
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.346	3.46 ug/L	325842	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	95
2	Heptanal	114	C7H14O	000111-71-7	95
3	Heptanal	114	C7H14O	000111-71-7	93
4	Heptanal	114	C7H14O	000111-71-7	90
5	Heptanal	114	C7H14O	000111-71-7	70



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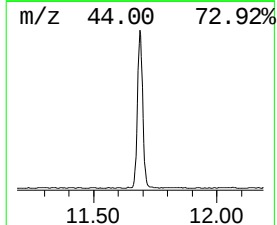
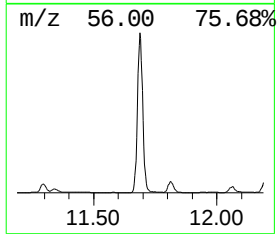
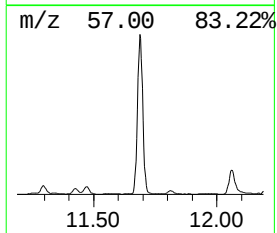
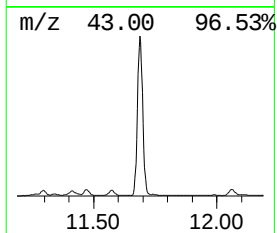
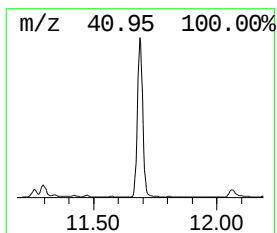
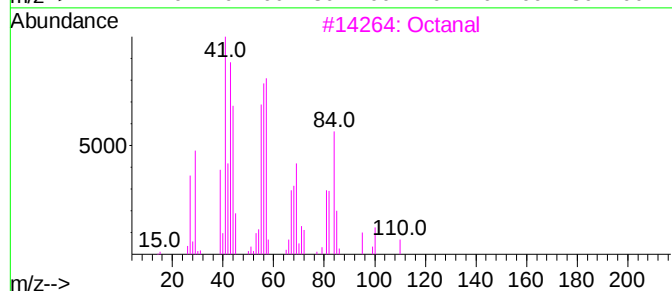
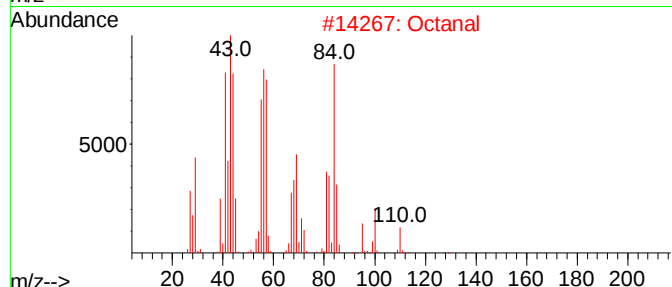
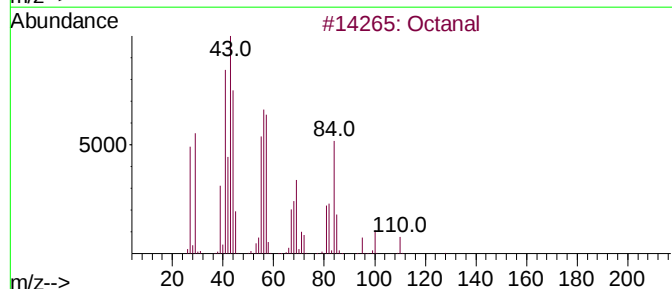
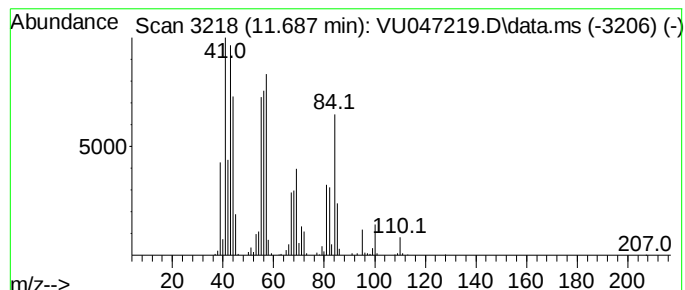
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 6 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	6.71 ug/L	732741	1,4-Dichlorobenzene-d4	11.812

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal		128	C8H16O	000124-13-0	97
2	Octanal		128	C8H16O	000124-13-0	96
3	Octanal		128	C8H16O	000124-13-0	91
4	Octanal		128	C8H16O	000124-13-0	90
5	Octanal		128	C8H16O	000124-13-0	47



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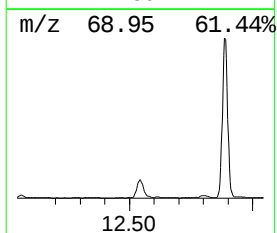
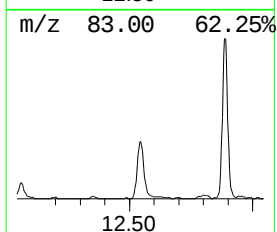
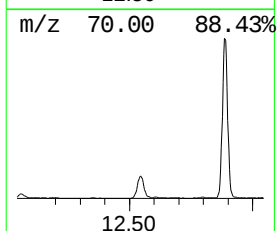
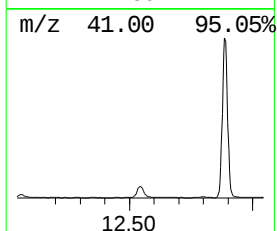
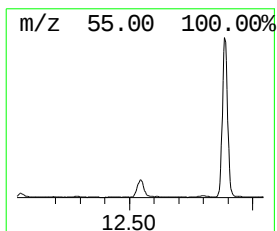
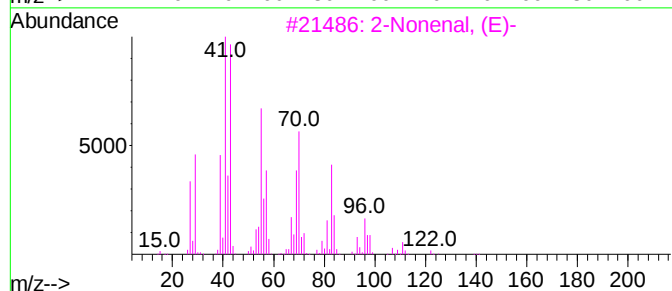
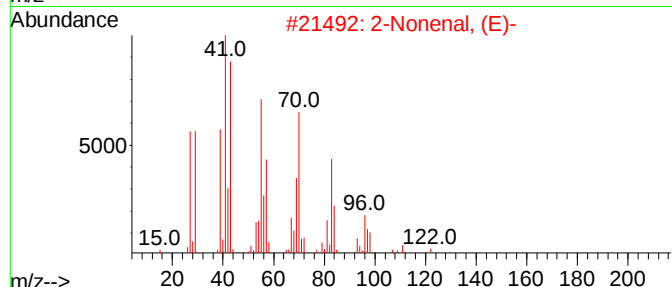
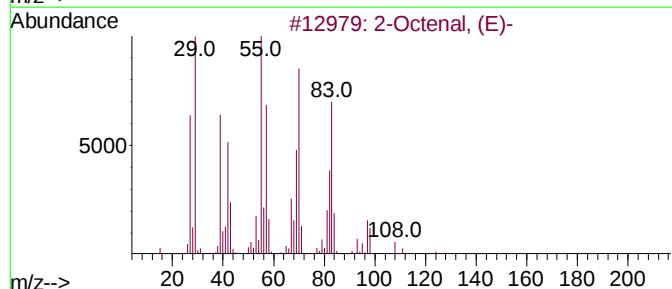
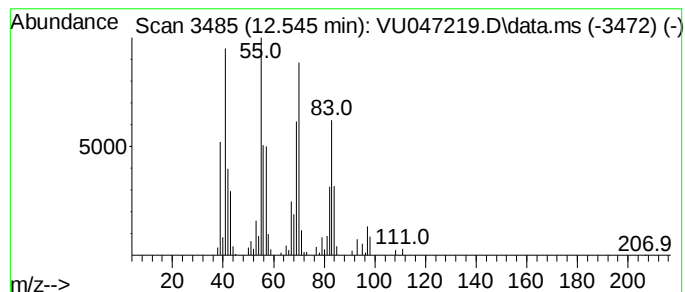
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 2-Octenal, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	1.28 ug/L	140181	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octenal, (E)-	126	C8H14O	002548-87-0	72
2	2-Nonenal, (E)-	140	C9H16O	018829-56-6	72
3	2-Nonenal, (E)-	140	C9H16O	018829-56-6	64
4	2-Octenal, (E)-	126	C8H14O	002548-87-0	64
5	2-Nonenal, (E)-	140	C9H16O	018829-56-6	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021822\
Data File : VU047219.D
Acq On : 17 Feb 2022 21:11
Operator : SY/MD
Sample : N1545-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY03

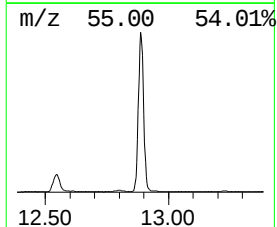
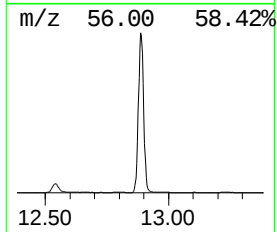
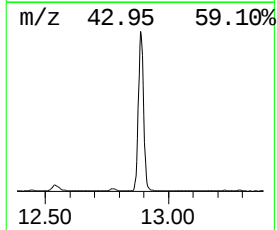
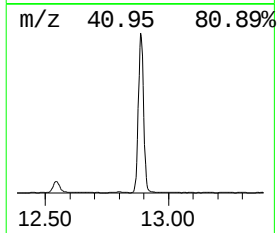
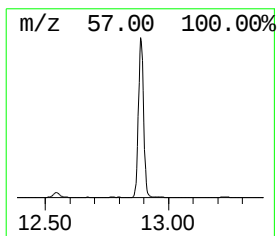
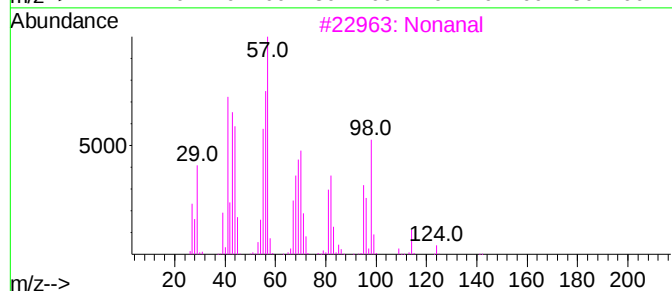
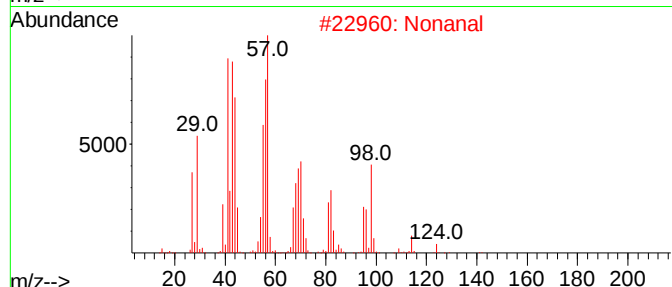
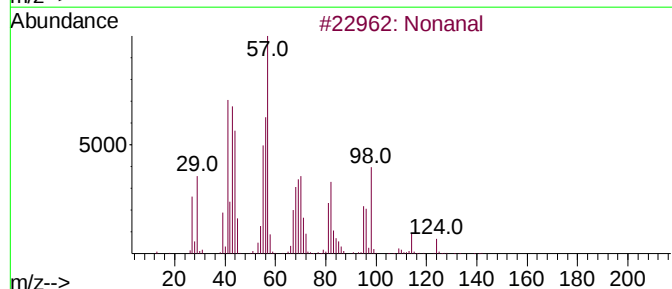
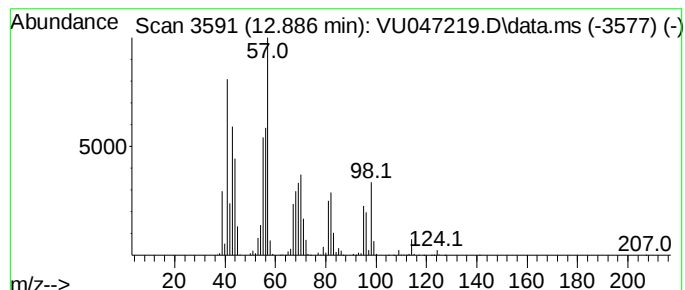
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Quant Title : TRACE VOA SFAM1.0

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	15.54 ug/L	1697060	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	90
3	Nonanal		142	C9H18O	000124-19-6	90
4	Nonanal		142	C9H18O	000124-19-6	72
5	Cyclohexanol, 2-methyl-, trans-		114	C7H14O	007443-52-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021822\
Data File : VU047219.D
Acq On : 17 Feb 2022 21:11
Operator : SY/MD
Sample : N1545-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY03

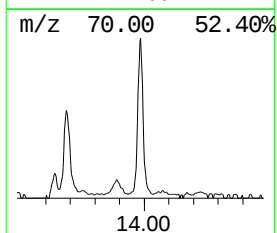
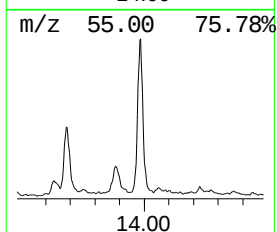
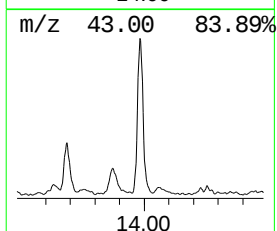
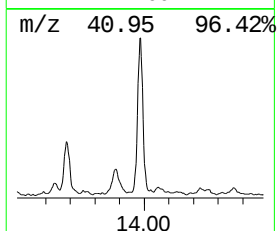
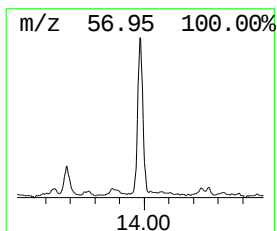
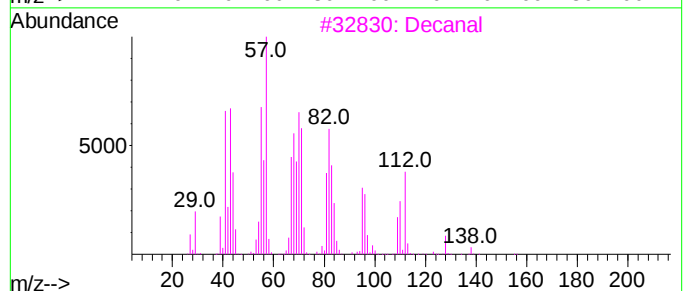
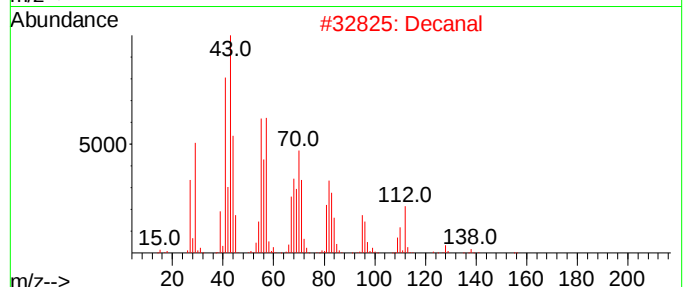
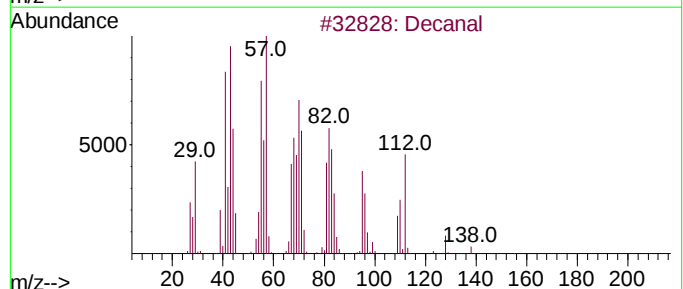
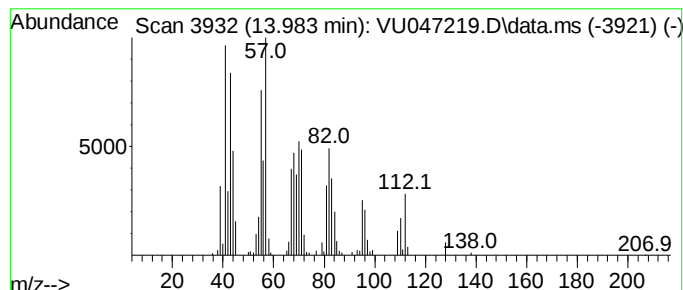
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Decanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.983	1.50 ug/L	163421	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanal	156	C10H20O	000112-31-2	91
2	Decanal	156	C10H20O	000112-31-2	91
3	Decanal	156	C10H20O	000112-31-2	87
4	Decanal	156	C10H20O	000112-31-2	87
5	2-Octen-1-ol, (E)-	128	C8H16O	018409-17-1	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021822\
Data File : VU047219.D
Acq On : 17 Feb 2022 21:11
Operator : SY/MD
Sample : N1545-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY03

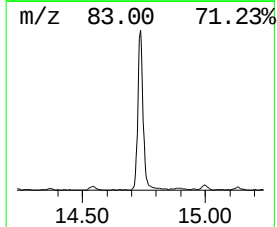
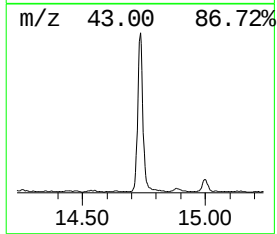
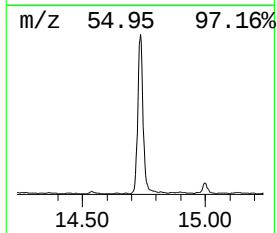
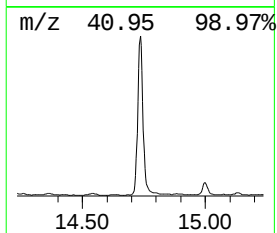
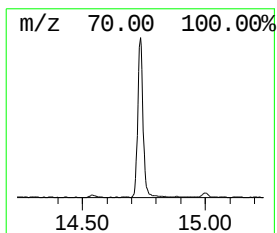
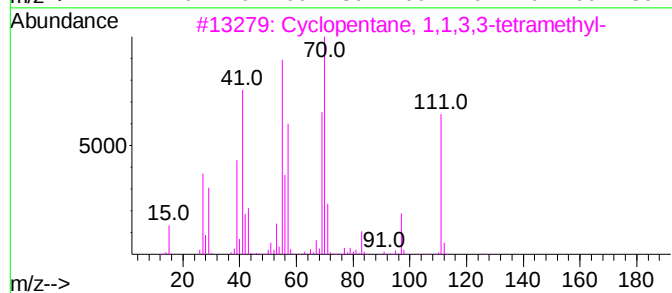
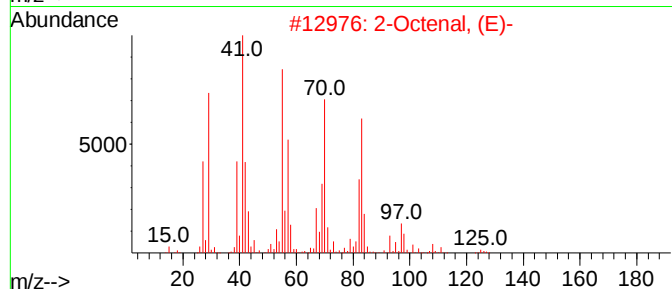
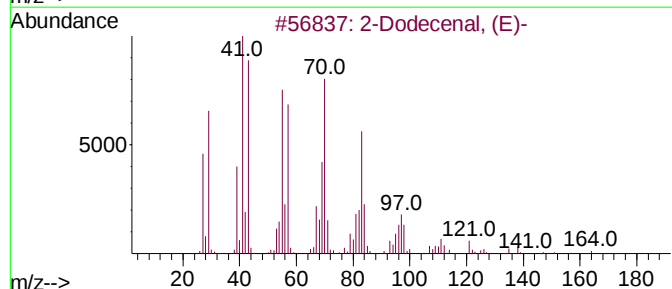
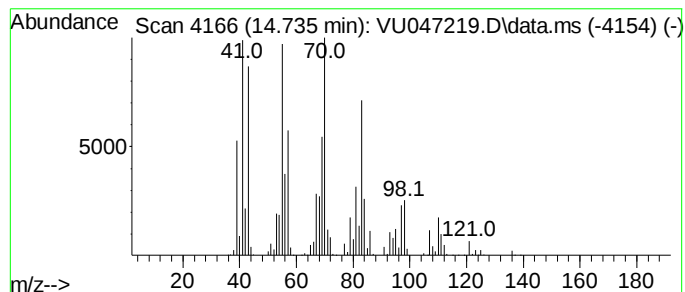
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	5.74 ug/L	627033	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Dodecenal, (E)-	182	C12H22O	020407-84-5	64
2	2-Octenal, (E)-	126	C8H14O	002548-87-0	50
3	Cyclopentane, 1,1,3,3-tetramethyl-	126	C9H18	050876-33-0	46
4	2-Hexenal, (E)-	98	C6H10O	006728-26-3	38
5	2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021822\
Data File : VU047219.D
Acq On : 17 Feb 2022 21:11
Operator : SY/MD
Sample : N1545-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY03

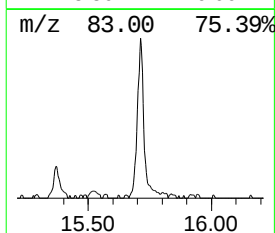
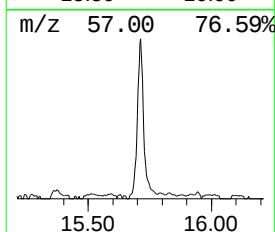
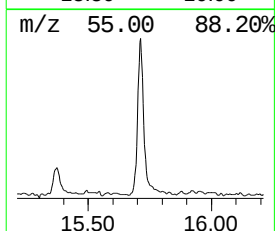
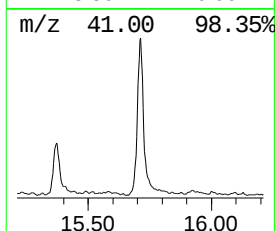
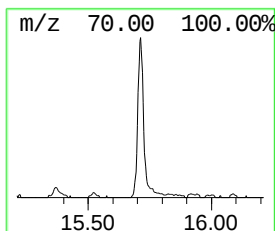
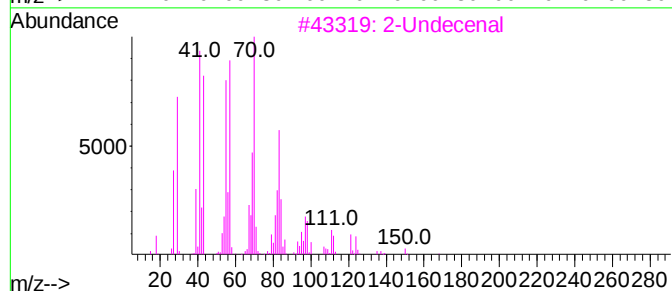
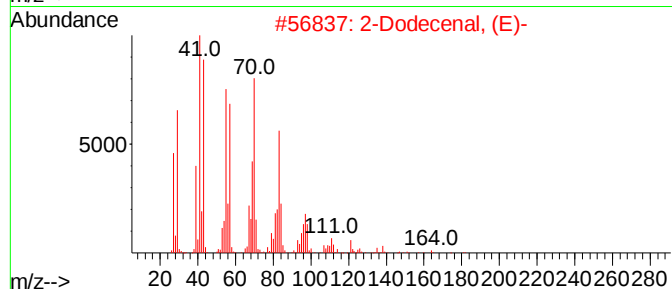
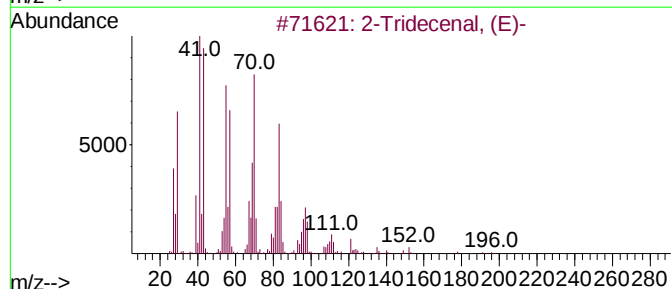
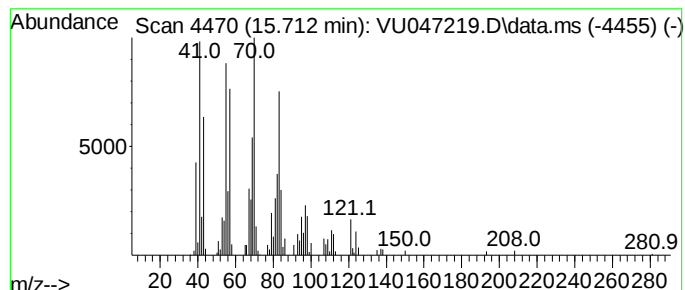
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2-Tridecenal, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.712	1.52 ug/L	166300	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	64
4	2-tert-Butyl-3,4,5,6-tetrahydrop...	139	C9H17N	090949-17-0	53
5	Isoheptadecanol	256	C17H36O	057289-07-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021822\
Data File : VU047219.D
Acq On : 17 Feb 2022 21:11
Operator : SY/MD
Sample : N1545-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY03

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.363	4.7	ug/L	318644	1	6.253	342268	5.0
Pentanal	6.880	2.3	ug/L	158527	1	6.253	342268	5.0
Hexanal	8.787	25.9	ug/L	2443630	2	9.420	471109	5.0
Heptanal	10.346	3.5	ug/L	325842	2	9.420	471109	5.0
Octanal	11.687	6.7	ug/L	732741	3	11.812	546142	5.0
2-Octenal, (E)-	12.545	1.3	ug/L	140181	3	11.812	546142	5.0
Nonanal	12.886	15.5	ug/L	1697060	3	11.812	546142	5.0
Decanal	13.983	1.5	ug/L	163421	3	11.812	546142	5.0
2-Dodecenal, (E)-	14.735	5.7	ug/L	627033	3	11.812	546142	5.0
2-Tridecenal, (E)-	15.712	1.5	ug/L	166300	3	11.812	546142	5.0