

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030822\
 Data File : VU047397.D
 Acq On : 08 Mar 2022 17:45
 Operator : SY/MD
 Sample : N1840-02DL 4X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFY21DL

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\SFAMUTR030422WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU047397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.362	3	7	21	rVB	89789	88521	8.58%	1.087%
2	1.600	68	81	95	rBV3	74777	115625	11.20%	1.420%
3	1.697	104	111	118	rBV	8546	12880	1.25%	0.158%
4	1.919	171	180	197	rBV	47517	66019	6.40%	0.811%
5	2.160	247	255	263	rBV2	10893	14314	1.39%	0.176%
6	2.211	263	271	287	rVB3	15235	24965	2.42%	0.307%
7	2.571	365	383	396	rBV2	83845	176094	17.06%	2.163%
8	2.655	399	409	424	rVB2	3990	11748	1.14%	0.144%
9	3.054	519	533	554	rVB2	9104	19665	1.91%	0.242%
10	3.369	614	631	654	rBV	78150	185427	17.97%	2.278%
11	4.456	956	969	987	rBV5	5316	14308	1.39%	0.176%
12	4.668	1010	1035	1075	rBV2	135681	528869	51.25%	6.496%
13	5.067	1144	1159	1177	rVB	95495	212304	20.57%	2.608%
14	5.729	1340	1365	1375	rBV2	173134	473344	45.87%	5.814%
15	6.250	1512	1527	1546	rBV	212773	399788	38.74%	4.911%
16	6.546	1605	1619	1635	rBV	82746	153979	14.92%	1.891%
17	6.693	1651	1665	1682	rBV	120989	237621	23.03%	2.919%
18	6.880	1711	1723	1754	rBV2	51363	113379	10.99%	1.393%
19	7.568	1922	1937	1951	rBV	63622	111247	10.78%	1.366%
20	7.899	2024	2040	2055	rBV	196193	339421	32.89%	4.169%
21	7.970	2055	2062	2075	rVB2	5940	10336	1.00%	0.127%
22	8.182	2117	2128	2139	rBV	39927	67318	6.52%	0.827%
23	8.555	2232	2244	2257	rVV	134805	225892	21.89%	2.775%
24	8.635	2257	2269	2303	rVV	425092	837664	81.17%	10.289%
25	8.787	2303	2316	2364	rVB	590459	1031967	100.00%	12.676%
26	9.417	2497	2512	2532	rBV	293930	495172	47.98%	6.082%
27	10.343	2789	2800	2823	rVB	102251	166771	16.16%	2.049%
28	10.758	2917	2929	2944	rVB	130231	211912	20.53%	2.603%
29	10.893	2960	2971	2981	rBV2	6585	10697	1.04%	0.131%
30	11.298	3090	3097	3105	rVB5	10539	16292	1.58%	0.200%
31	11.471	3143	3151	3160	rVB4	7469	12134	1.18%	0.149%
32	11.687	3207	3218	3240	rBV	185988	282646	27.39%	3.472%
33	11.812	3245	3257	3272	rVB	349152	552378	53.53%	6.785%
34	12.195	3363	3376	3391	rBV	250607	405847	39.33%	4.985%
35	12.545	3474	3485	3497	rBV4	17714	31634	3.07%	0.389%
36	12.886	3578	3591	3616	rBV	265048	393576	38.14%	4.834%

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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\SFAMUTR030422WMA.M
Title : TRACE VOA SFAM1.0

37	13.687	3831	3840	3854	rBV3	8805	13668	1.32%	0.168%
38	13.983	3922	3932	3946	rVB3	14621	21731	2.11%	0.267%
39	14.735	4156	4166	4183	rBV4	22764	35565	3.45%	0.437%
40	16.886	4828	4835	4846	rBV3	12403	18365	1.78%	0.226%

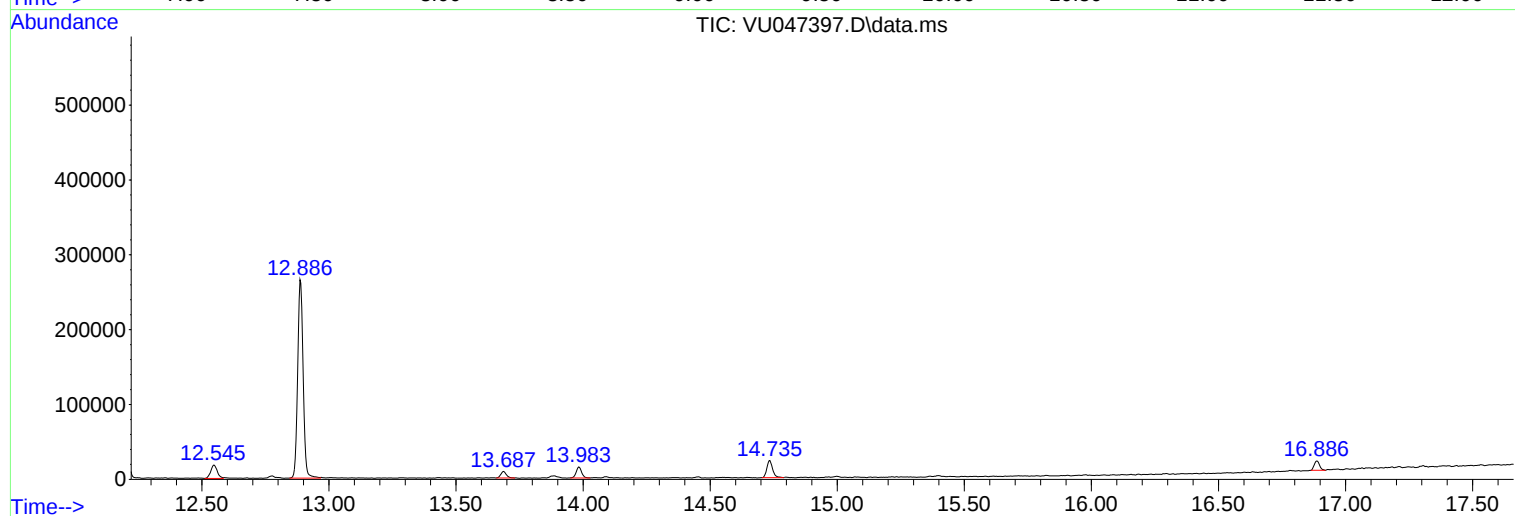
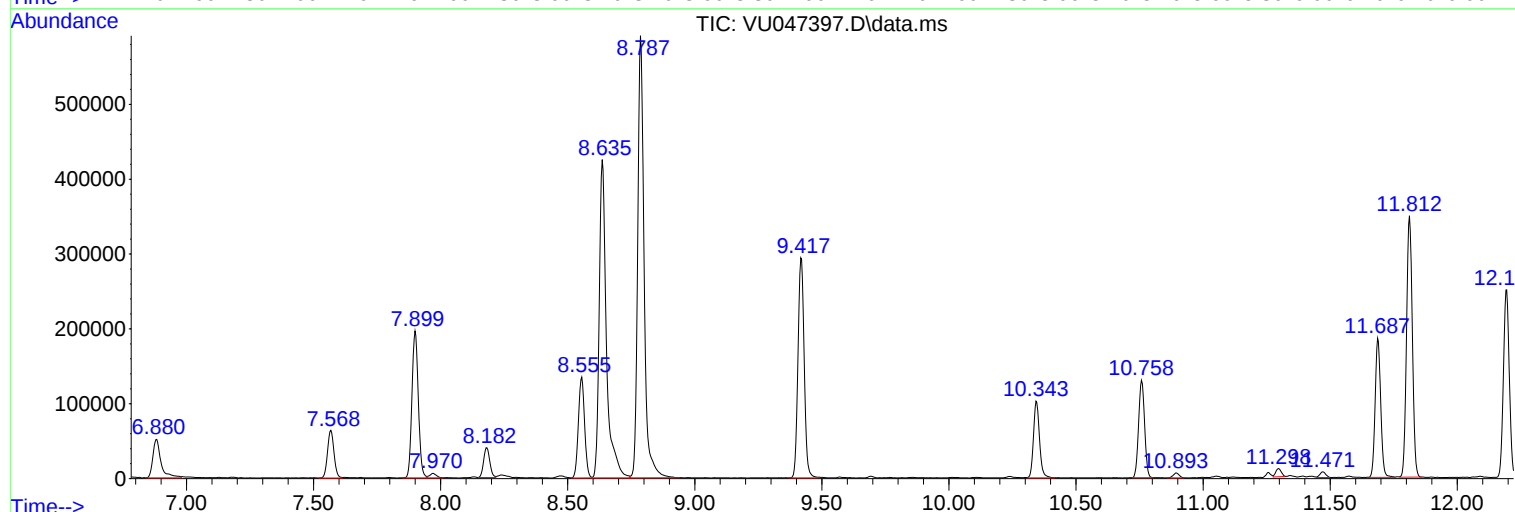
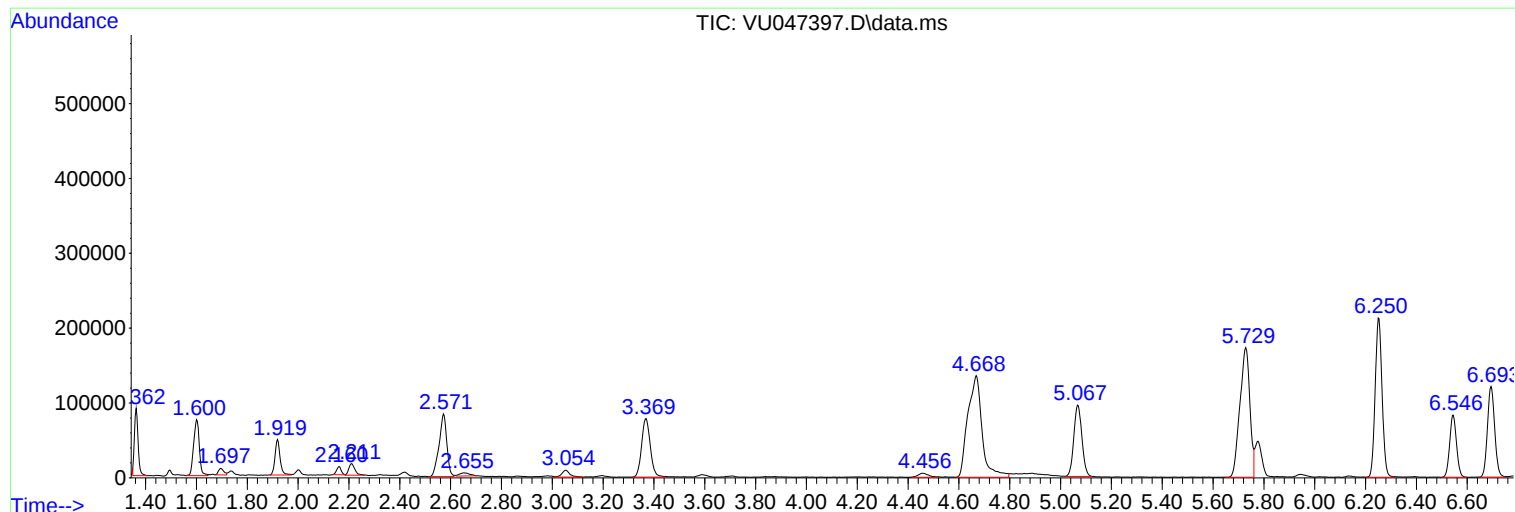
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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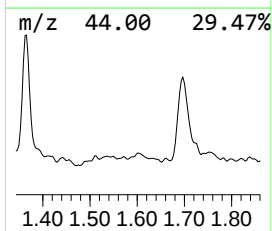
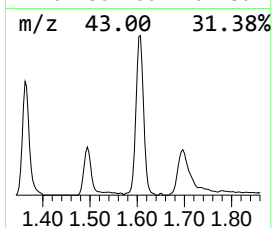
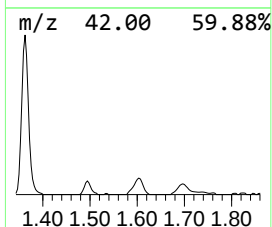
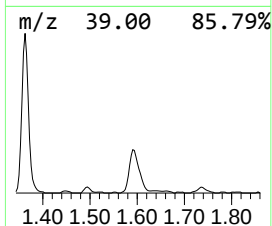
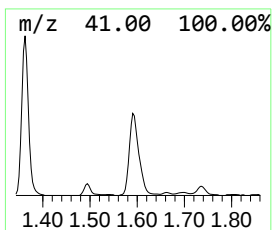
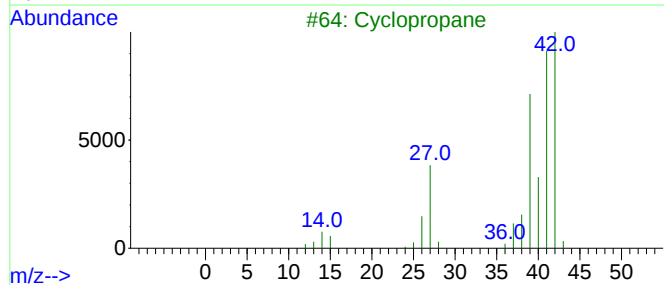
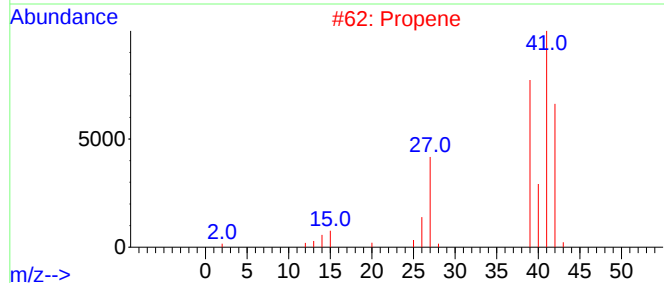
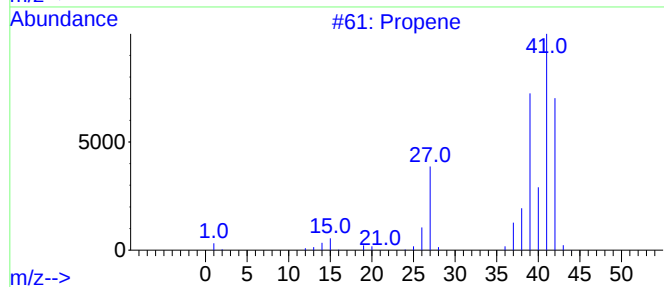
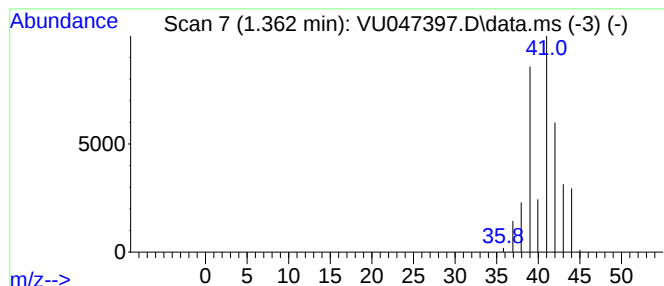
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.362	1.11 ug/L	88521	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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Instrument :
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ClientSampleId :
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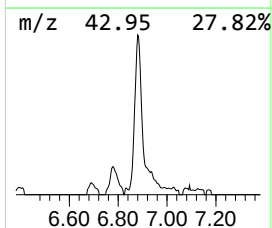
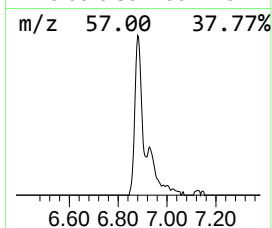
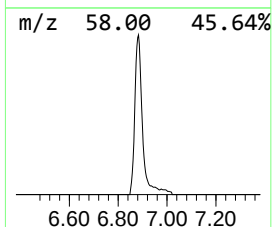
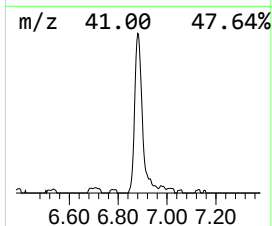
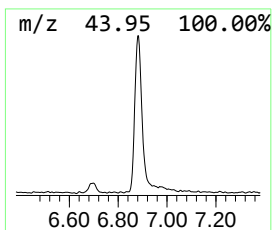
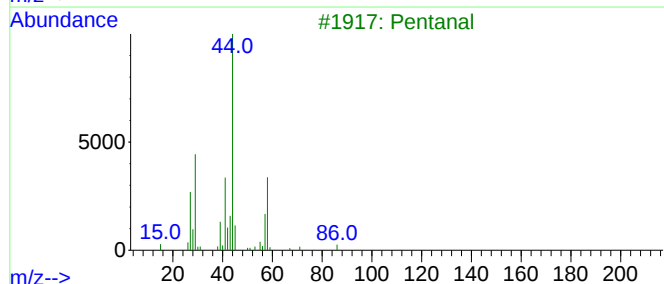
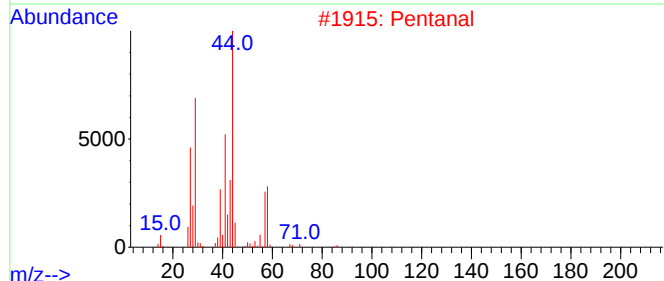
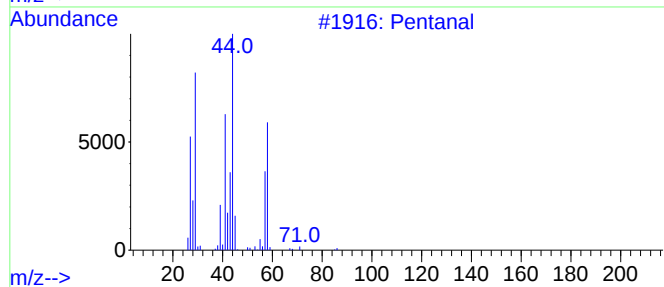
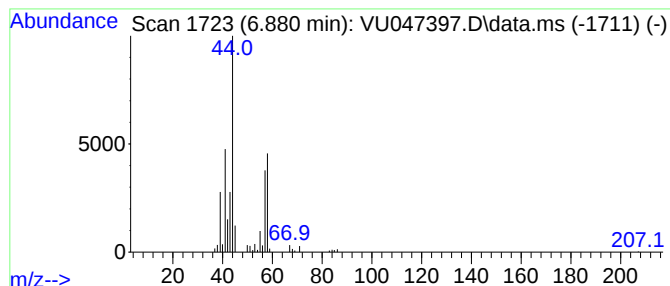
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	1.42 ug/L	113379	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentanal	86	C5H10O	000110-62-3	90
2		Pentanal	86	C5H10O	000110-62-3	90
3		Pentanal	86	C5H10O	000110-62-3	83
4		Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
5		Butanal, 3-methyl-	86	C5H10O	000590-86-3	64



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Instrument :
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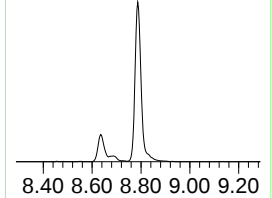
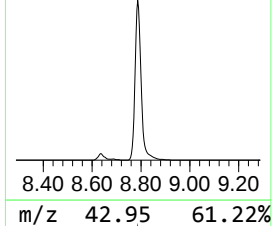
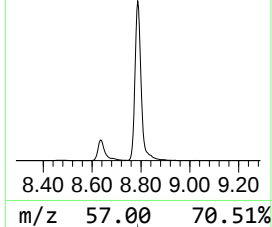
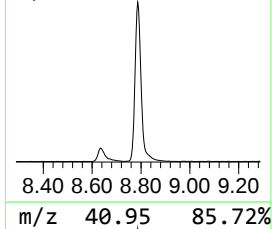
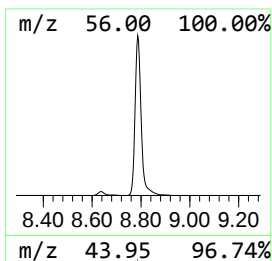
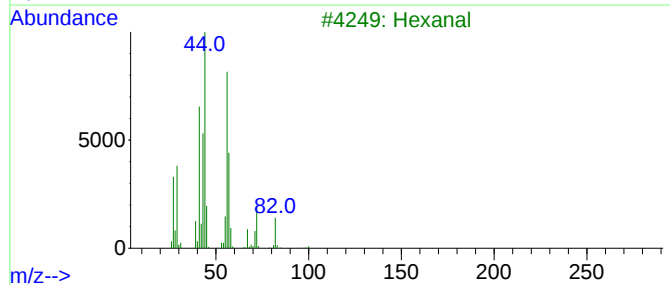
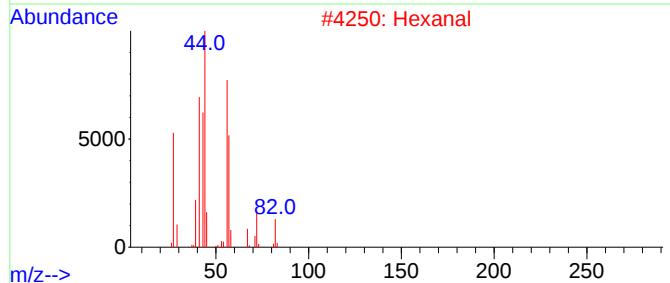
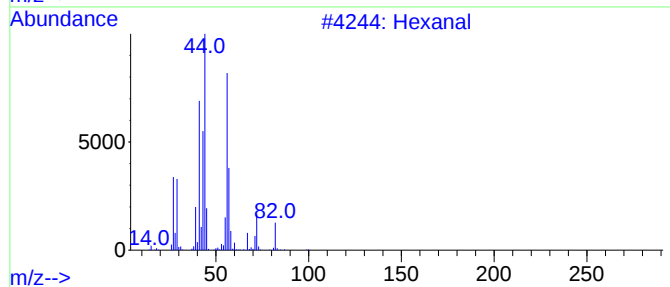
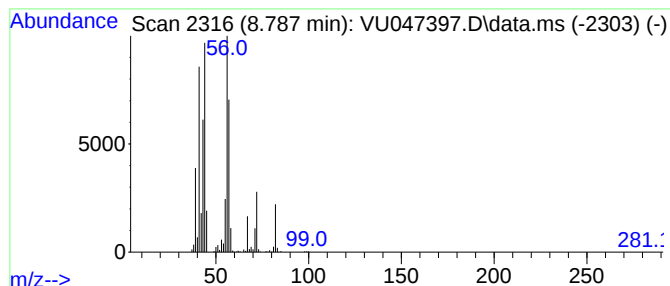
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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	10.42 ug/L	1031970	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	80
2	Hexanal			100	C6H12O	000066-25-1	80
3	Hexanal			100	C6H12O	000066-25-1	74
4	Hexanal			100	C6H12O	000066-25-1	72
5	Glutaraldehyde			100	C5H8O2	000111-30-8	38



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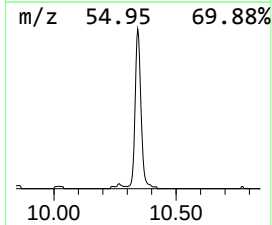
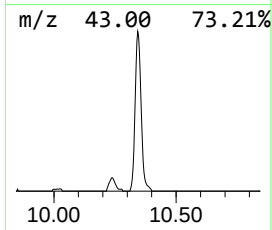
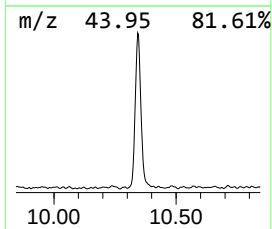
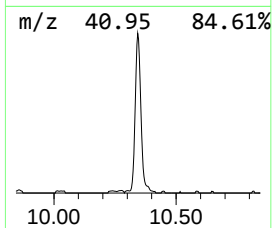
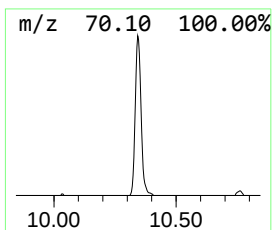
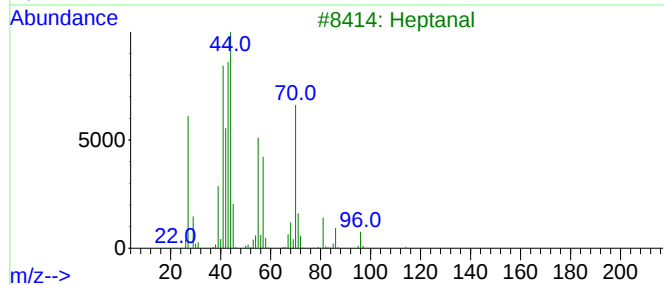
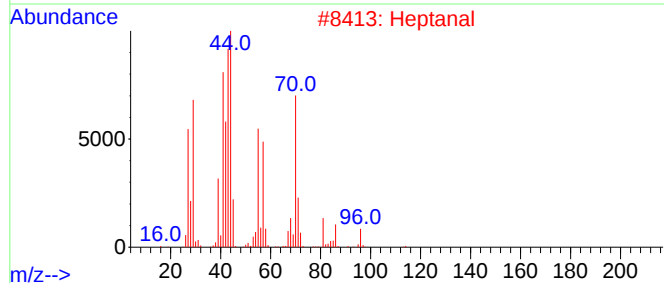
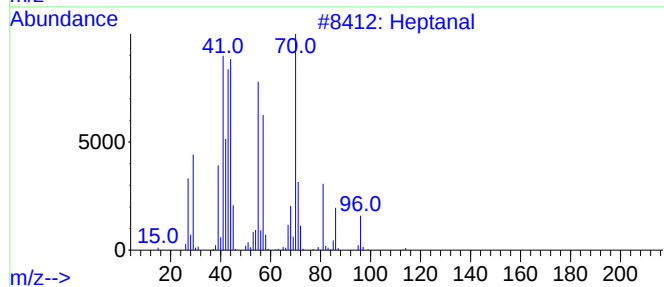
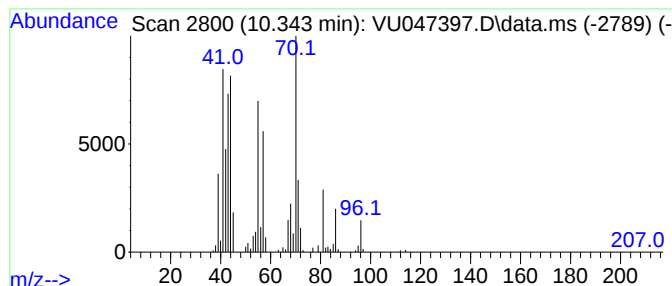
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.343	1.68 ug/L	166771	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	96
2			Heptanal	114	C7H14O	000111-71-7	96
3			Heptanal	114	C7H14O	000111-71-7	95
4			Heptanal	114	C7H14O	000111-71-7	58
5			Heptanal	114	C7H14O	000111-71-7	46



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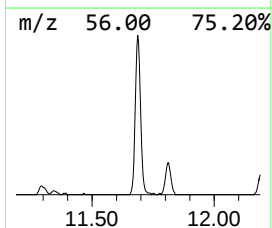
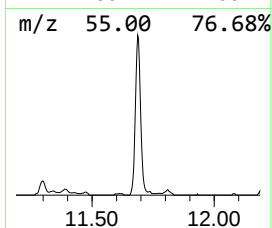
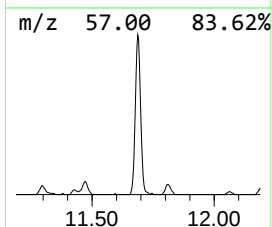
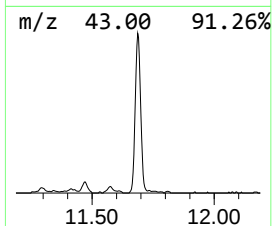
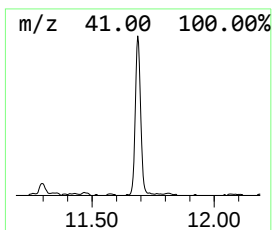
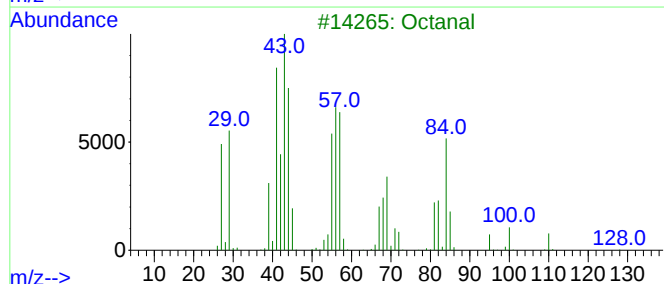
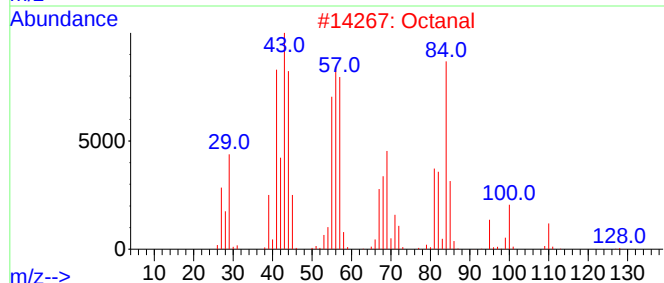
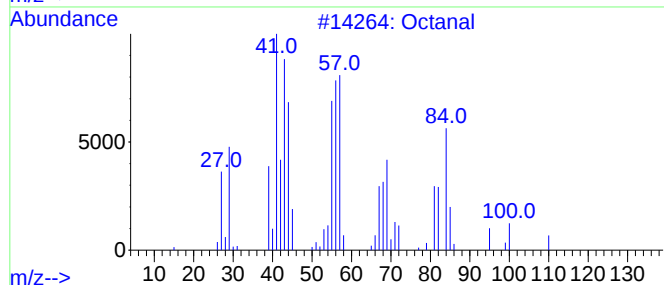
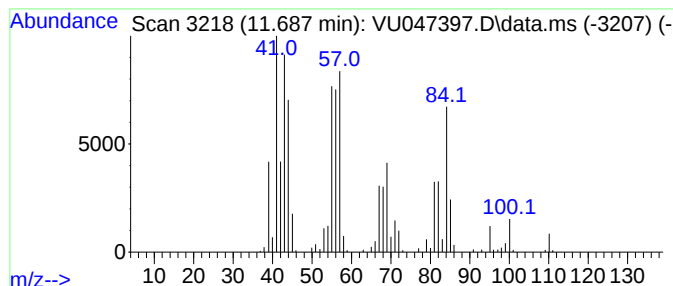
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.M
Quant Title : TRACE VOA SFAM1.0

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	2.56 ug/L	282646	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	91
3	Octanal			128	C8H16O	000124-13-0	90
4	Octanal			128	C8H16O	000124-13-0	86
5	Octanal			128	C8H16O	000124-13-0	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030822\
Data File : VU047397.D
Acq On : 08 Mar 2022 17:45
Operator : SY/MD
Sample : N1840-02DL 4X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY21DL

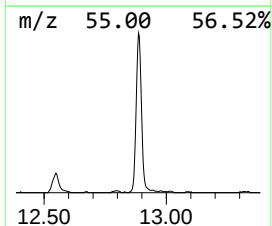
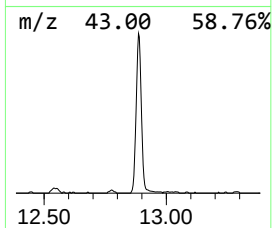
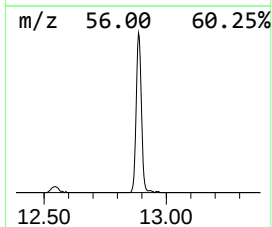
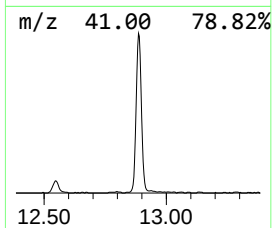
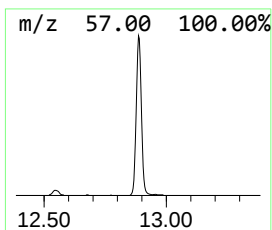
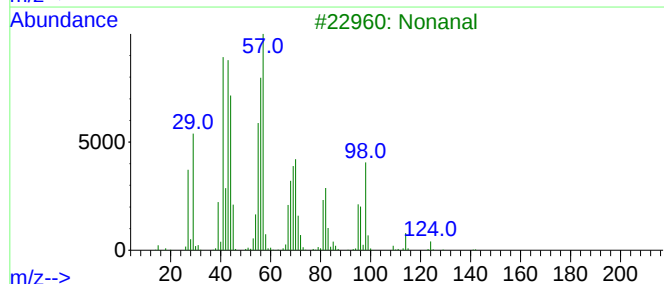
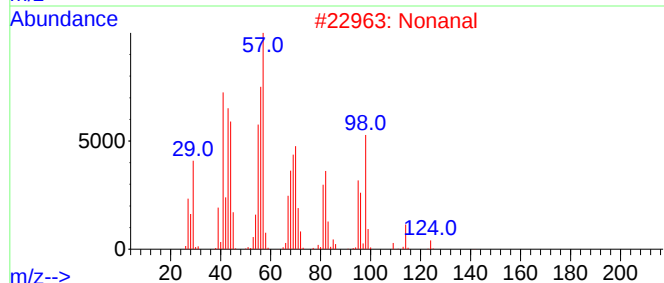
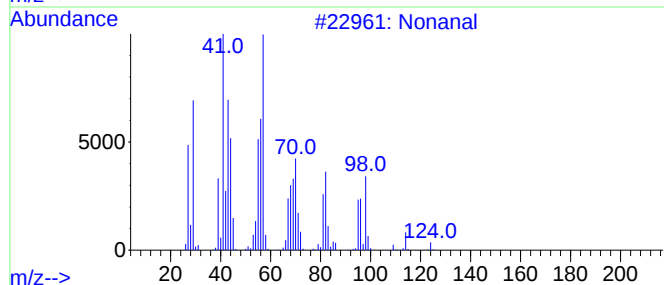
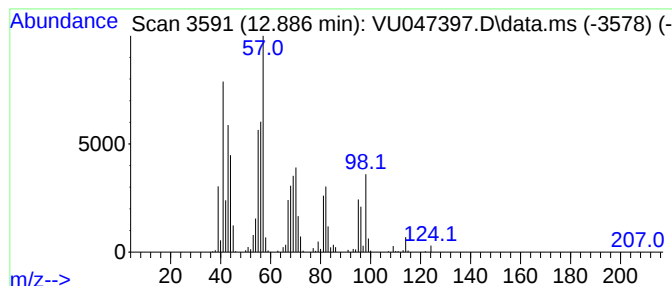
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	3.56 ug/L	393576	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	83
4			Nonanal	142	C9H18O	000124-19-6	72
5			Cyanoacetic acid, heptyl ester	183	C10H17NO2	1000406-22-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030822\
Data File : VU047397.D
Acq On : 08 Mar 2022 17:45
Operator : SY/MD
Sample : N1840-02DL 4X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY21DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030422WMA.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...	1.362	1.1	ug/L	88521	1	6.250	399788	5.0
Pentanal	6.880	1.4	ug/L	113379	1	6.250	399788	5.0
Hexanal	8.787	10.4	ug/L	1031970	2	9.417	495172	5.0
Heptanal	10.343	1.7	ug/L	166771	2	9.417	495172	5.0
Octanal	11.687	2.6	ug/L	282646	3	11.812	552378	5.0
Nonanal	12.886	3.6	ug/L	393576	3	11.812	552378	5.0