

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
 Data File : VU047413.D
 Acq On : 09 Mar 2022 18:45
 Operator : SY/MD
 Sample : N1840-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFY22

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\SFAMUTR030922WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU047413.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	24	rVB	164316	161799	9.72%	1.401%
2	1.597	70	80	91	rBV3	121988	210371	12.63%	1.822%
3	1.697	104	111	118	rBV2	12722	19435	1.17%	0.168%
4	1.736	118	123	138	rVB3	14831	19842	1.19%	0.172%
5	1.919	171	180	196	rVB	45290	62827	3.77%	0.544%
6	2.160	246	255	262	rBV	19534	26092	1.57%	0.226%
7	2.211	262	271	290	rVB3	43820	77164	4.63%	0.668%
8	2.417	326	335	347	rVB6	9593	17521	1.05%	0.152%
9	2.581	367	386	402	rBV4	192627	423873	25.46%	3.671%
10	3.369	613	631	659	rBV	80629	190015	11.41%	1.645%
11	3.877	765	789	812	rBV	168411	406705	24.43%	3.522%
12	4.456	953	969	992	rBV3	9966	28537	1.71%	0.247%
13	4.668	1014	1035	1070	rBV3	69717	245165	14.72%	2.123%
14	5.070	1144	1160	1185	rBV	75061	182104	10.94%	1.577%
15	5.321	1224	1238	1256	rVB2	26771	58046	3.49%	0.503%
16	5.729	1344	1365	1380	rBV2	156377	398415	23.93%	3.450%
17	6.253	1513	1528	1545	rBV	201021	379209	22.77%	3.284%
18	6.542	1603	1618	1639	rVB3	99422	192306	11.55%	1.665%
19	6.694	1650	1665	1685	rBV2	92031	191138	11.48%	1.655%
20	6.880	1709	1723	1758	rBV	101544	214774	12.90%	1.860%
21	7.568	1922	1937	1950	rBV2	51248	89379	5.37%	0.774%
22	7.899	2025	2040	2054	rBV	209032	359414	21.59%	3.112%
23	7.970	2055	2062	2075	rVB2	9889	16782	1.01%	0.145%
24	8.182	2118	2128	2138	rBV	29423	47888	2.88%	0.415%
25	8.555	2232	2244	2257	rVB2	83957	141502	8.50%	1.225%
26	8.636	2257	2269	2289	rBV	199724	377690	22.68%	3.271%
27	8.787	2304	2316	2334	rBV	1014291	1665034	100.00%	14.419%
28	9.417	2500	2512	2532	rBV	278057	464479	27.90%	4.022%
29	9.693	2588	2598	2611	rBV	11865	20325	1.22%	0.176%
30	10.343	2785	2800	2829	rBV	383286	613992	36.88%	5.317%
31	10.758	2918	2929	2943	rBV	74966	121055	7.27%	1.048%
32	10.893	2959	2971	2983	rBV	29581	48804	2.93%	0.423%
33	11.256	3072	3084	3089	rBV	21453	31548	1.89%	0.273%
34	11.295	3089	3096	3107	rVB2	39369	62833	3.77%	0.544%
35	11.388	3117	3125	3132	rBV	22498	33070	1.99%	0.286%
36	11.468	3143	3150	3164	rVB4	11869	19696	1.18%	0.171%

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030922WMA.M
 Title : TRACE VOA SFAM1.0

37	11.687	3204	3218	3245	rBV	637069	948434	56.96%	8.213%
38	11.812	3245	3257	3276	rVB	327775	519213	31.18%	4.496%
39	12.192	3364	3375	3387	rBV	201745	324409	19.48%	2.809%
40	12.545	3474	3485	3501	rBV2	57540	104176	6.26%	0.902%
41	12.774	3544	3556	3574	rBV4	9369	23851	1.43%	0.207%
42	12.886	3577	3591	3615	rBV	1085257	1596262	95.87%	13.823%
43	13.684	3829	3839	3856	rVB2	40531	63040	3.79%	0.546%
44	13.893	3892	3904	3917	rVB8	7478	16885	1.01%	0.146%
45	13.983	3917	3932	3944	rBV4	13079	22764	1.37%	0.197%
46	14.735	4152	4166	4186	rBV	191845	309763	18.60%	2.682%

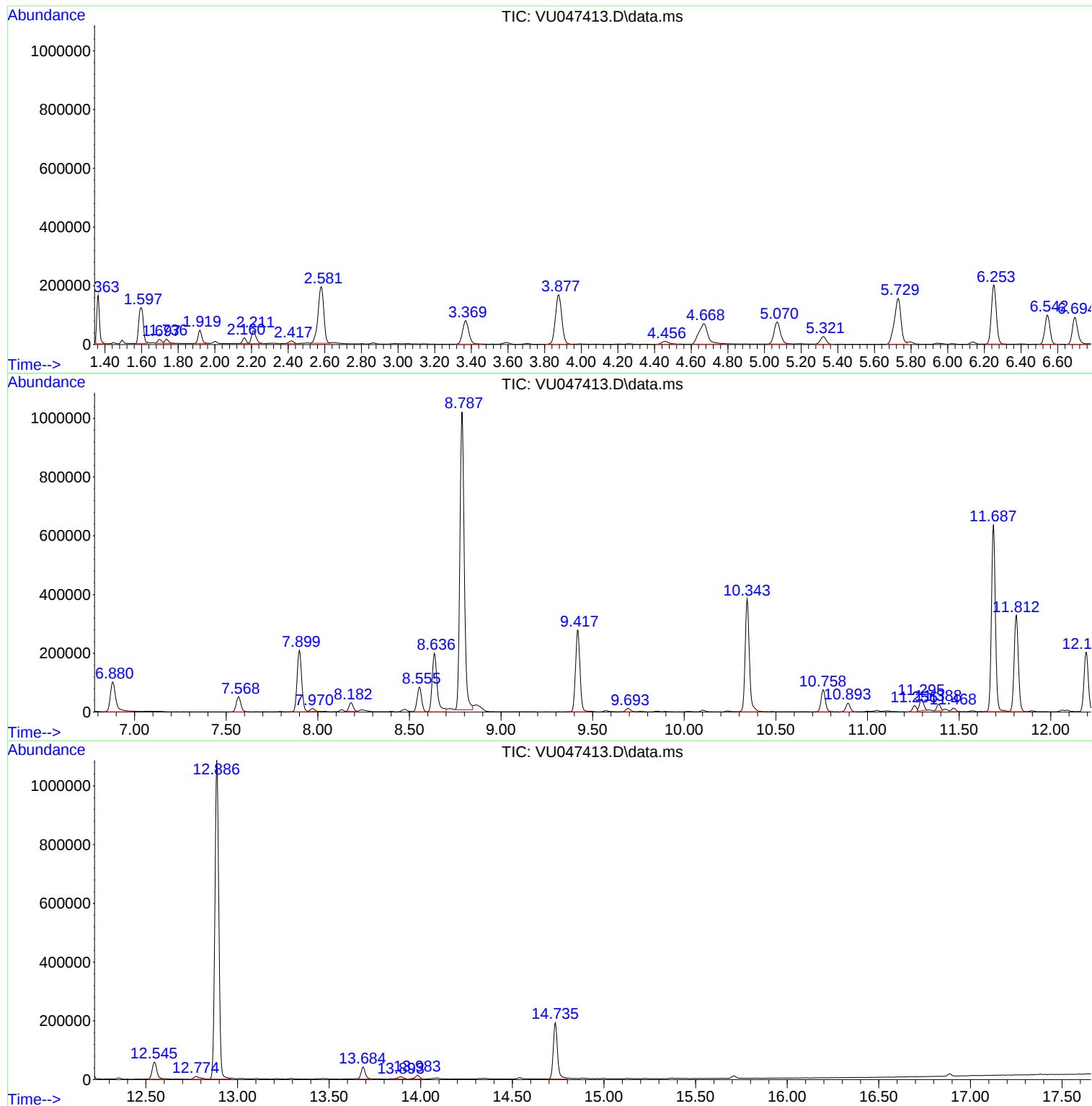
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030922WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY22

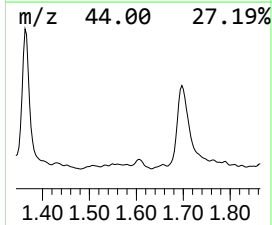
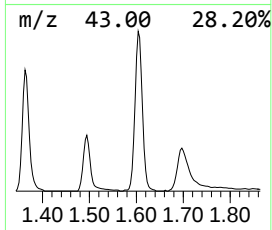
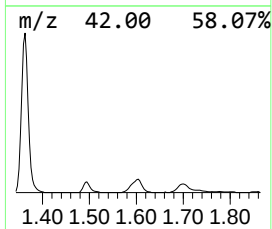
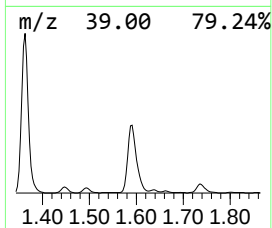
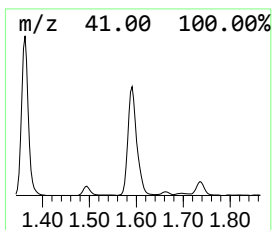
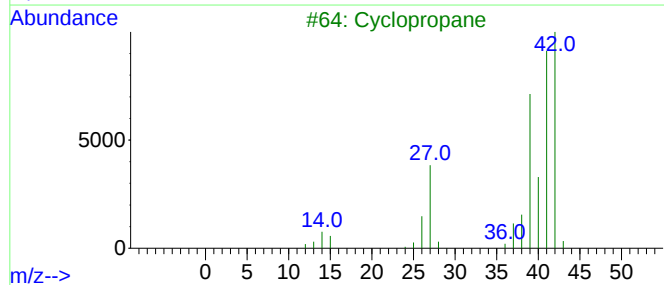
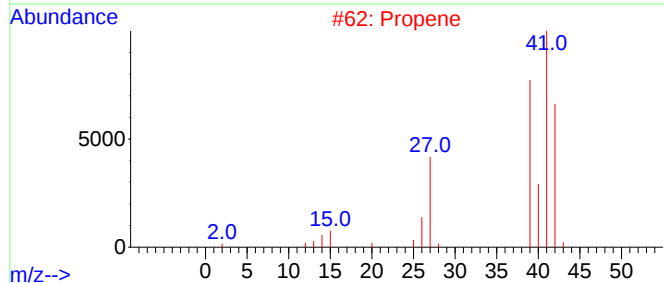
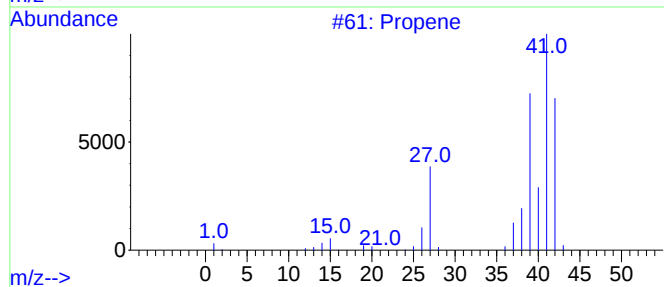
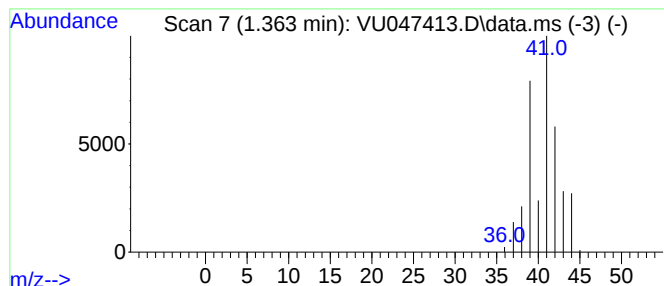
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.363	2.13 ug/L	161799	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	9
4			Cyclopropene	40	C3H4	002781-85-3	9
5			Cyclopropane	42	C3H6	000075-19-4	7



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY22

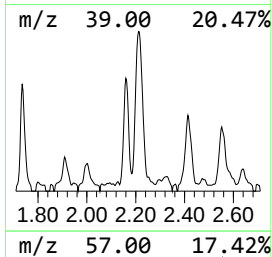
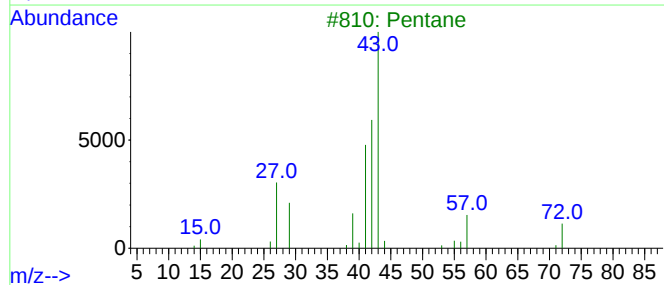
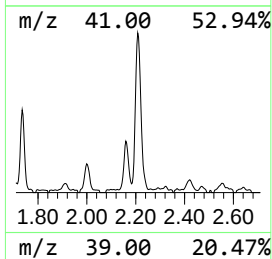
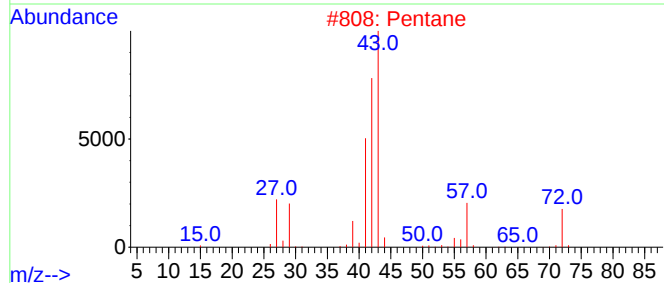
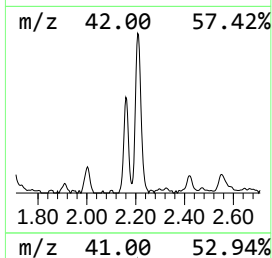
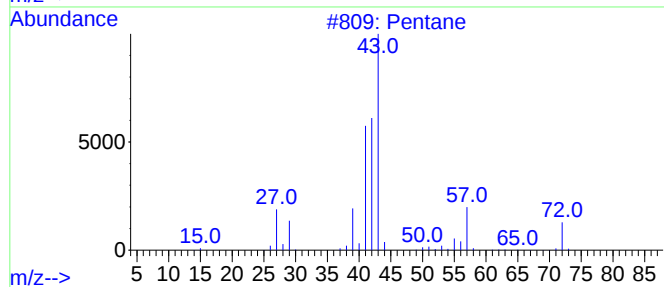
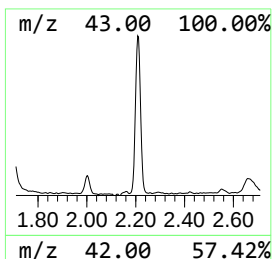
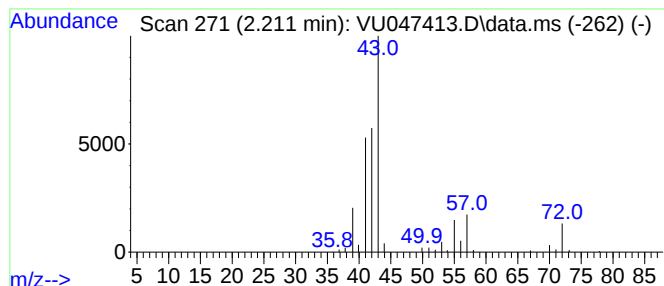
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.211	1.02 ug/L	77164	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	91
2	Pentane			72	C5H12	000109-66-0	86
3	Pentane			72	C5H12	000109-66-0	86
4	Pentane			72	C5H12	000109-66-0	86
5	Pentane			72	C5H12	000109-66-0	78



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Operator : SY/MD
Sample : N1840-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY22

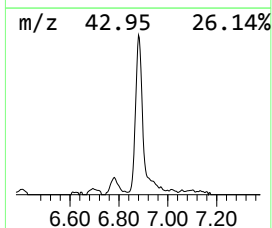
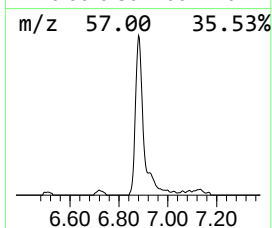
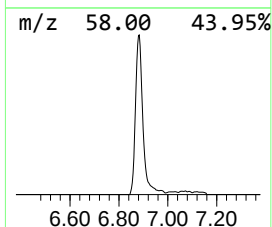
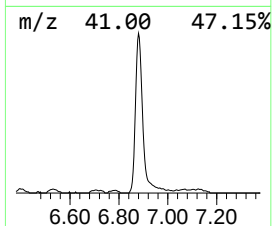
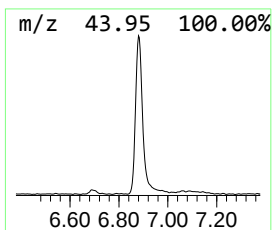
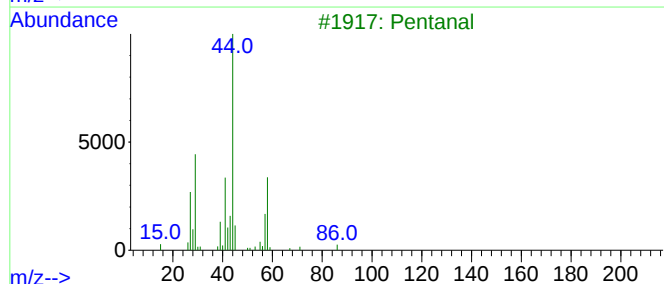
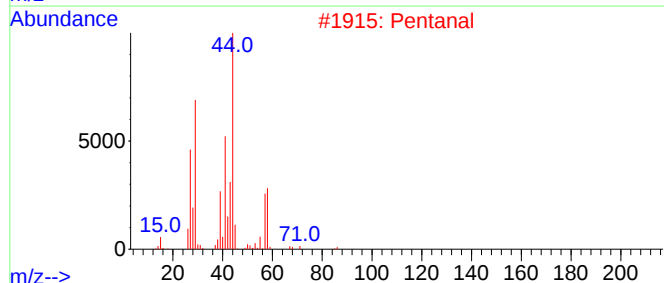
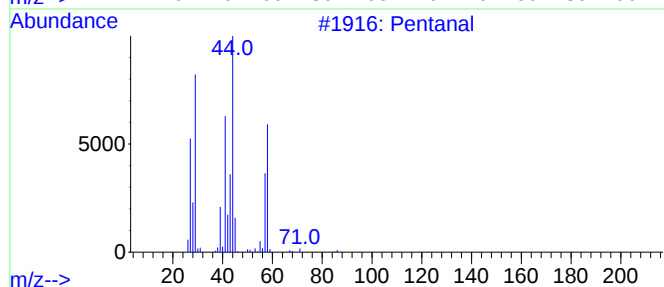
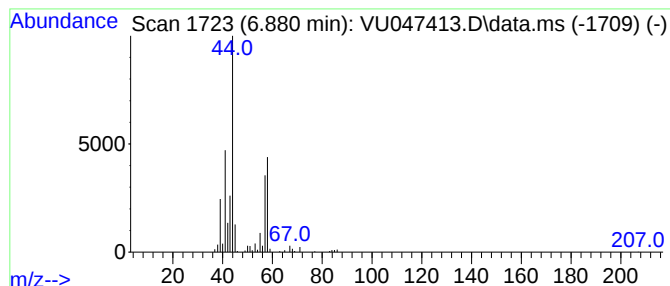
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	2.83 ug/L	214774	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	90
3	Pentanal			86	C5H10O	000110-62-3	90
4	Butanal, 3-methyl-			86	C5H10O	000590-86-3	83
5	Butanal, 3-methyl-			86	C5H10O	000590-86-3	78



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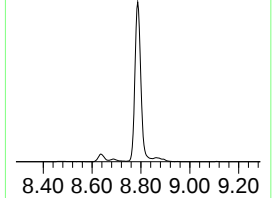
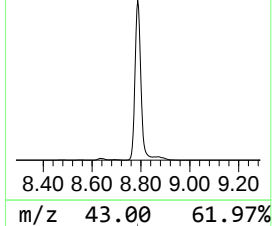
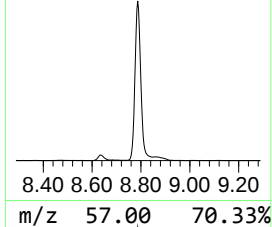
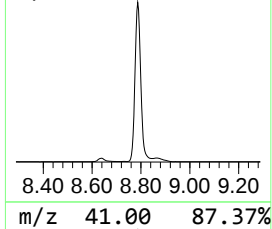
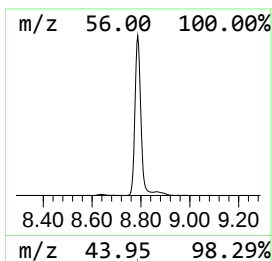
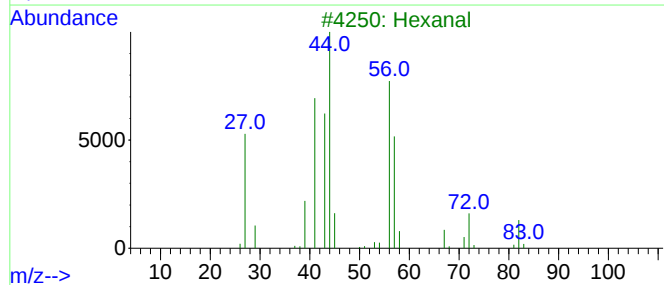
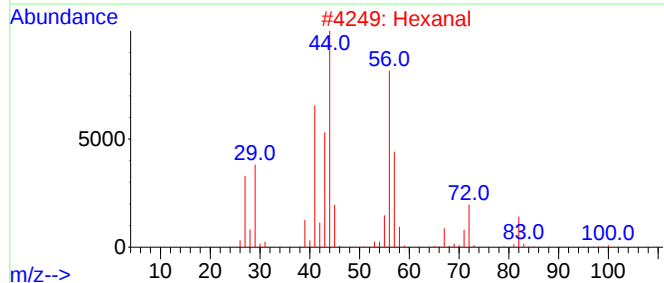
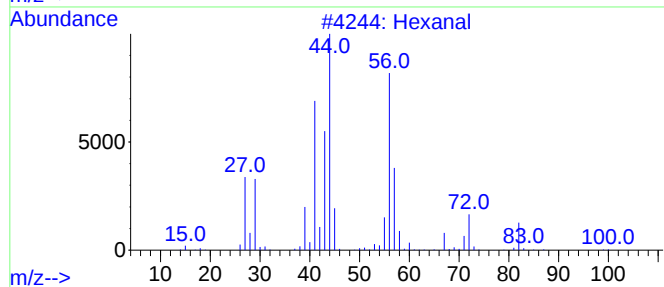
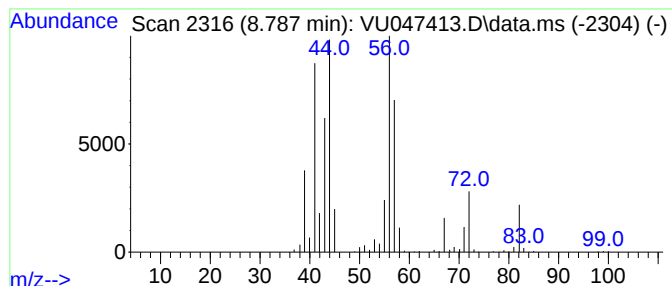
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	17.92 ug/L	1665030	Chlorobenzene-d5	9.420

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



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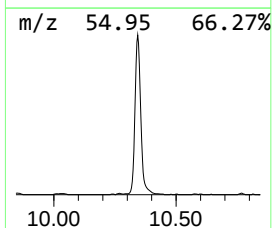
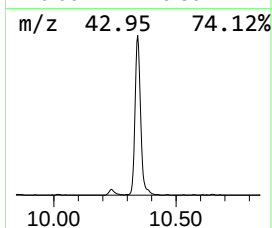
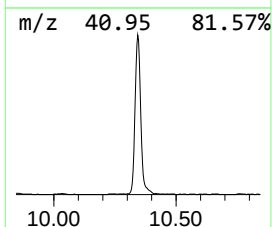
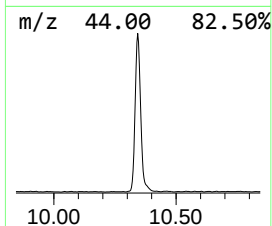
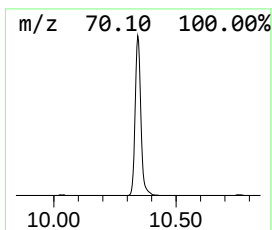
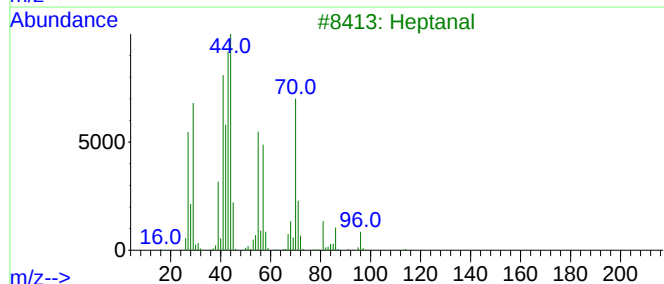
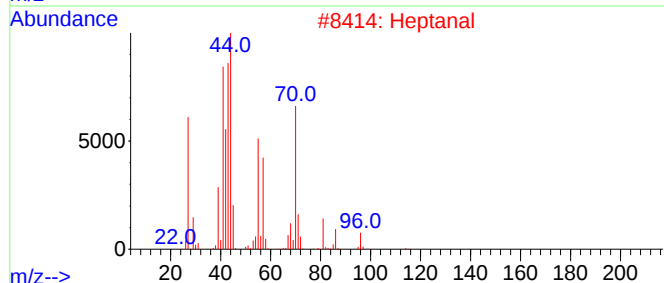
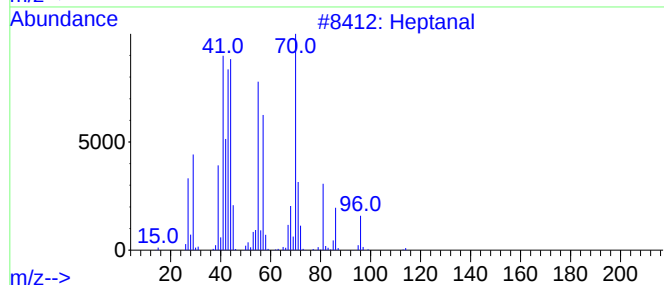
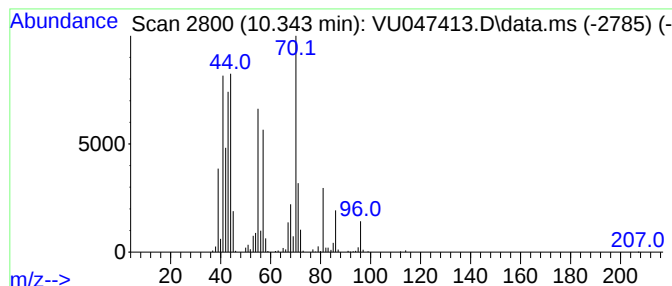
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030922WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.343	6.61 ug/L	613992	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	98
2	Heptanal			114	C7H14O	000111-71-7	94
3	Heptanal			114	C7H14O	000111-71-7	93
4	Heptanal			114	C7H14O	000111-71-7	64
5	Heptanal			114	C7H14O	000111-71-7	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
Data File : VU047413.D
Acq On : 09 Mar 2022 18:45
Operator : SY/MD
Sample : N1840-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY22

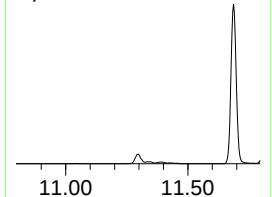
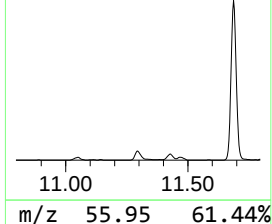
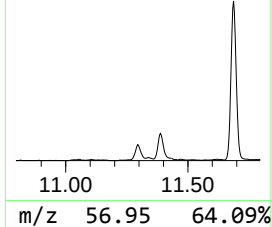
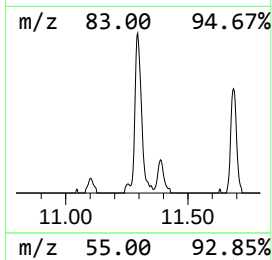
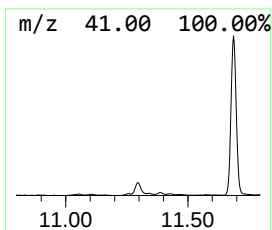
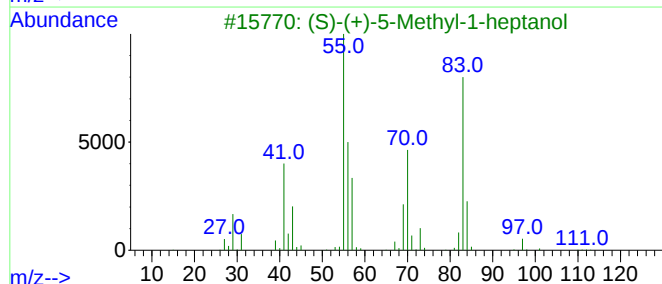
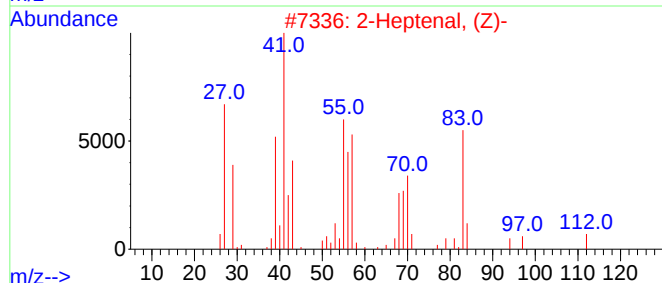
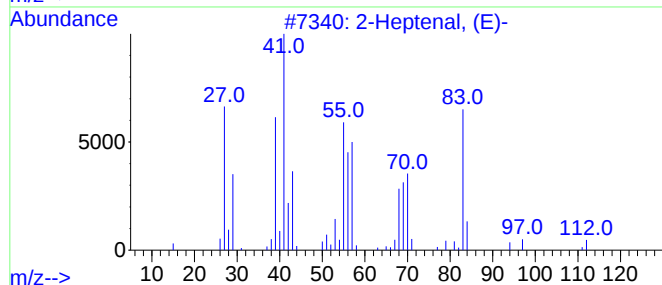
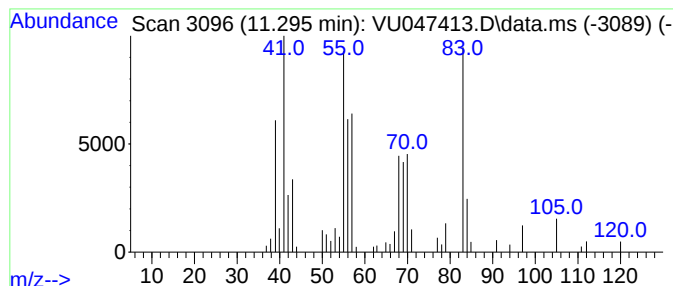
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 2-Heptenal, (E)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.295	0.61 ug/L	62833	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptenal, (E)-	112	C7H12O	018829-55-5	87
2			2-Heptenal, (Z)-	112	C7H12O	057266-86-1	87
3			(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	47
4			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	46
5			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
Data File : VU047413.D
Acq On : 09 Mar 2022 18:45
Operator : SY/MD
Sample : N1840-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY22

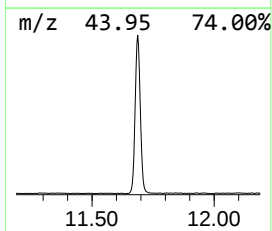
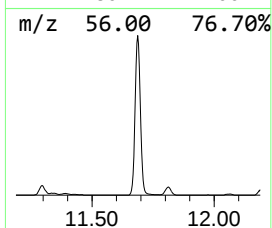
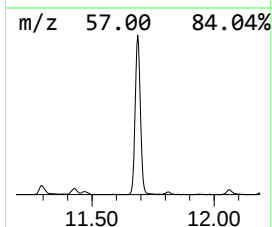
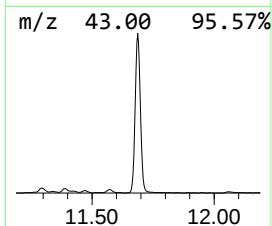
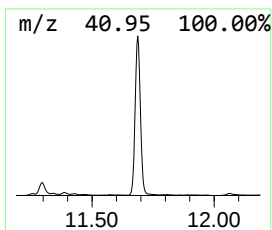
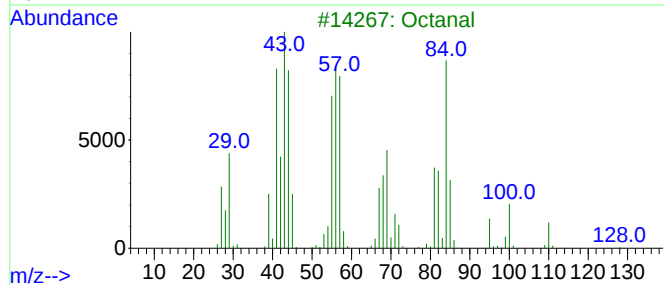
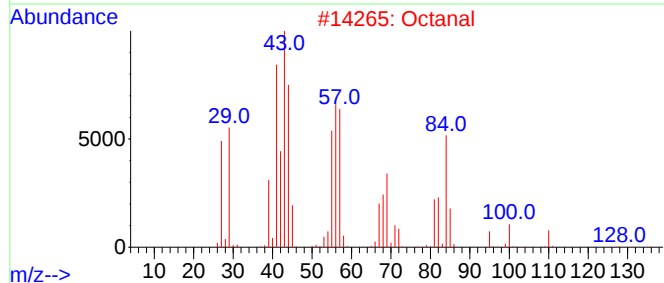
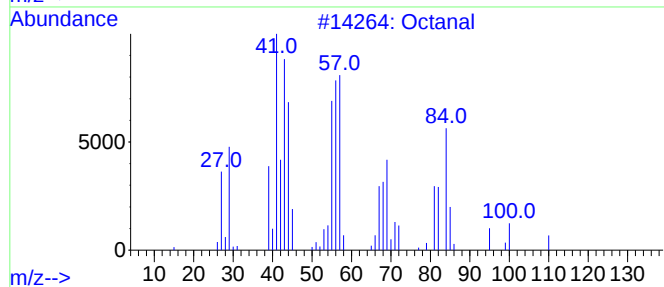
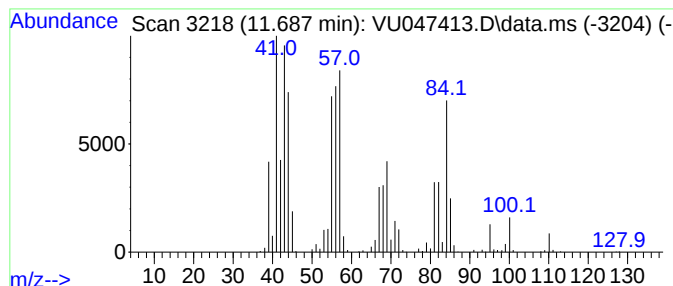
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	9.13 ug/L	948434	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	90
5	Octanal			128	C8H16O	000124-13-0	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
Data File : VU047413.D
Acq On : 09 Mar 2022 18:45
Operator : SY/MD
Sample : N1840-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY22

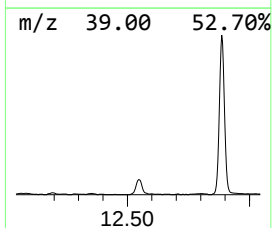
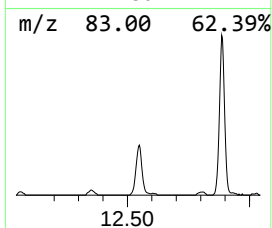
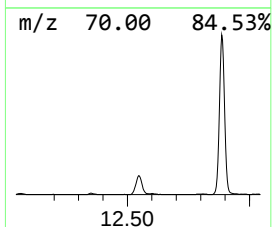
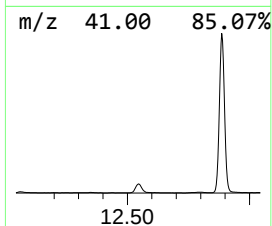
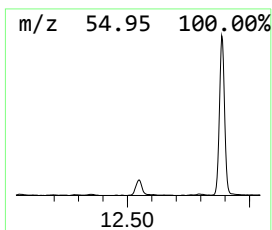
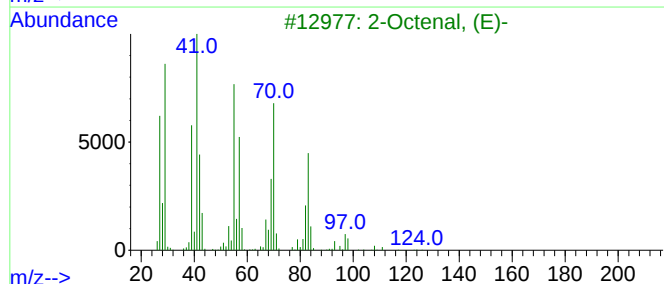
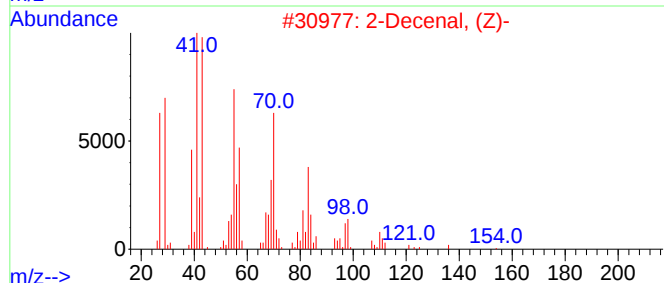
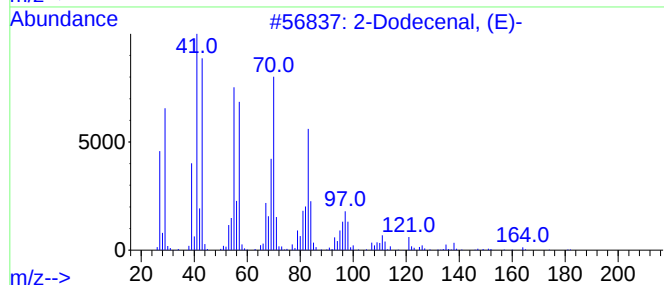
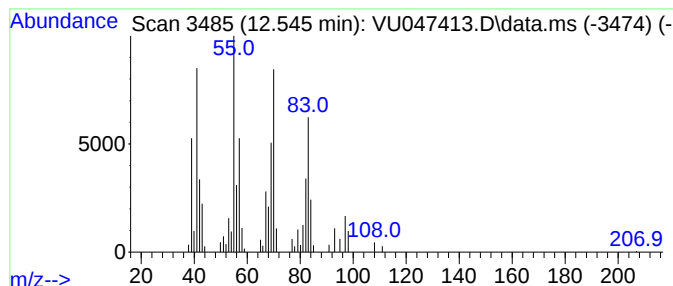
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 2-Dodecenal, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	1.00 ug/L	104176	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	72
2			2-Decenal, (Z)-	154	C10H18O	002497-25-8	59
3			2-Octenal, (E)-	126	C8H14O	002548-87-0	59
4			2-Nonenal, (Z)-	140	C9H16O	060784-31-8	53
5			Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
Data File : VU047413.D
Acq On : 09 Mar 2022 18:45
Operator : SY/MD
Sample : N1840-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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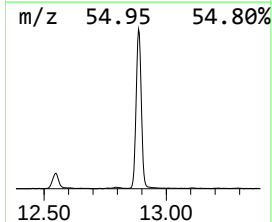
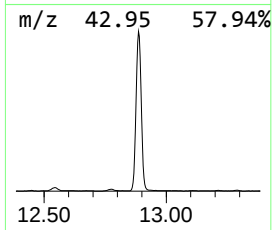
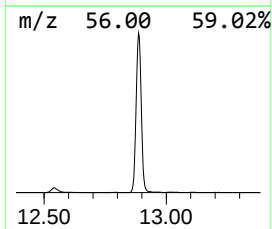
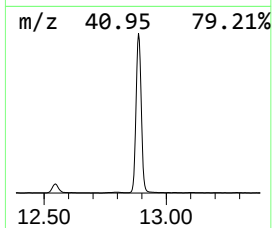
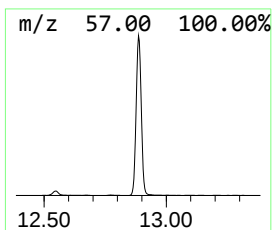
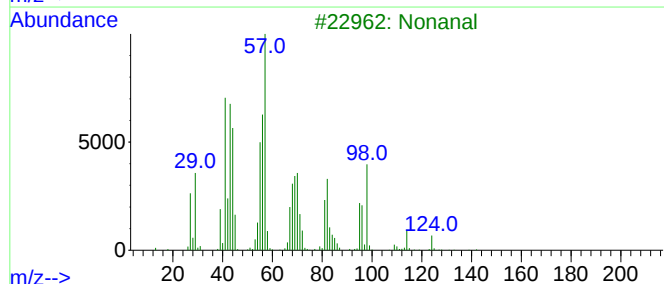
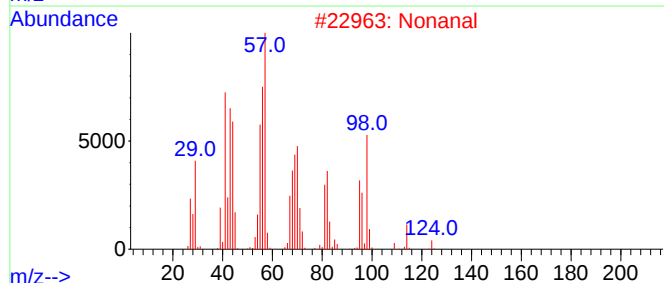
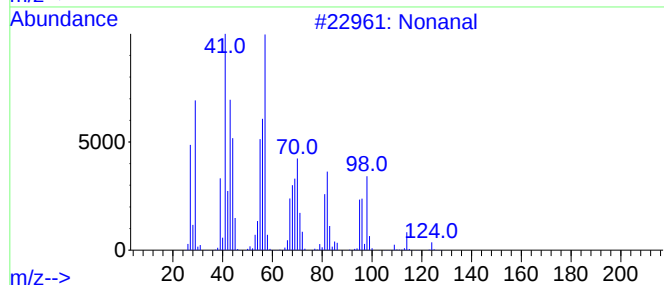
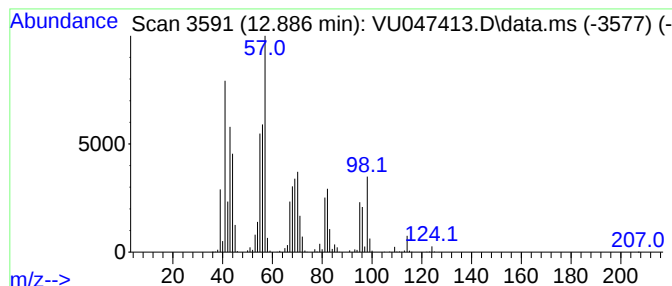
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	15.37 ug/L	1596260	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	90
5			5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
Data File : VU047413.D
Acq On : 09 Mar 2022 18:45
Operator : SY/MD
Sample : N1840-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFY22

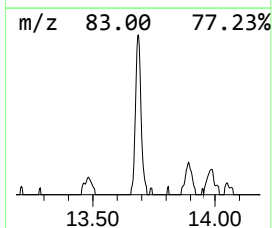
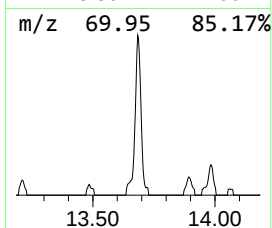
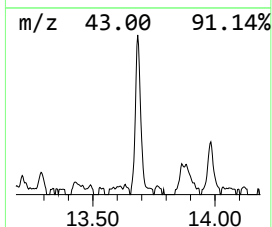
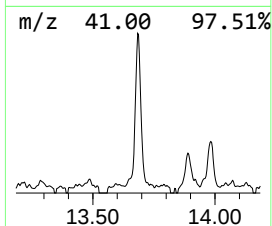
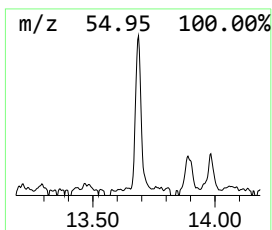
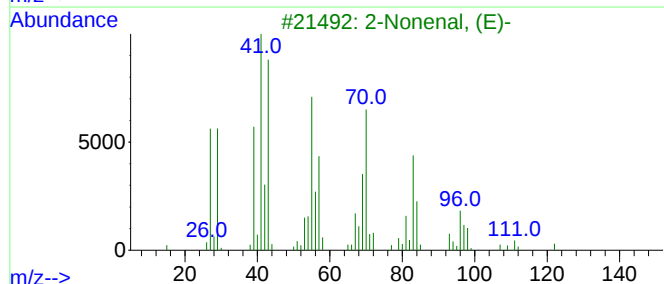
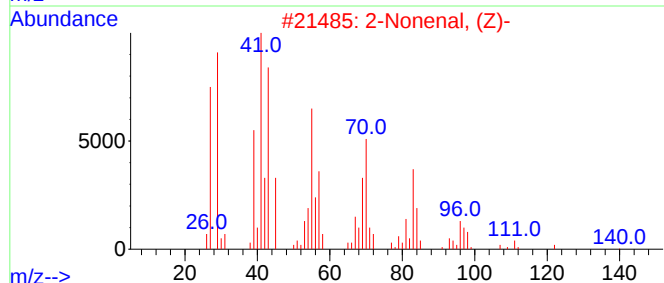
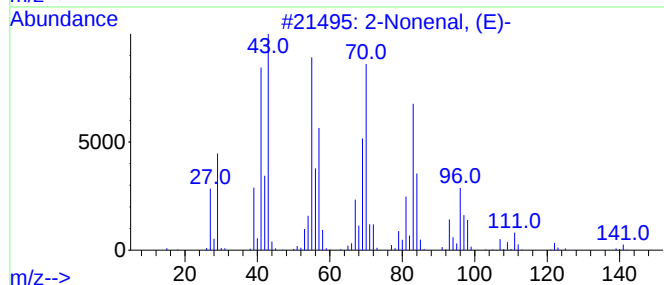
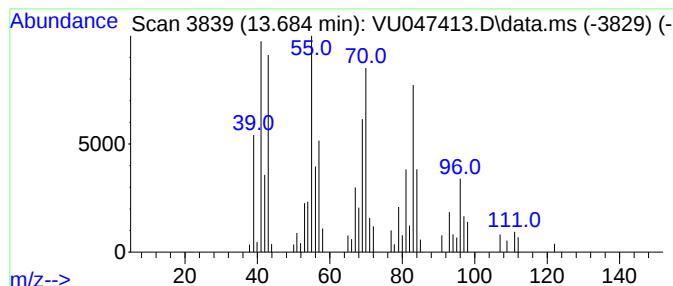
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2-Nonenal, (E)- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.684	0.61 ug/L	63040	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonenal, (E)-	140	C9H16O	018829-56-6	87
2			2-Nonenal, (Z)-	140	C9H16O	060784-31-8	78
3			2-Nonenal, (E)-	140	C9H16O	018829-56-6	78
4			2-Decenal, (E)-	154	C10H18O	003913-81-3	50
5			3-Undecene, 5-methyl-	168	C12H24	1000061-84-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
Data File : VU047413.D
Acq On : 09 Mar 2022 18:45
Operator : SY/MD
Sample : N1840-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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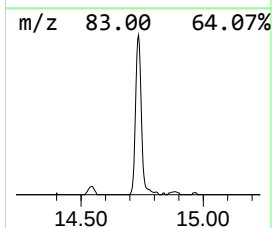
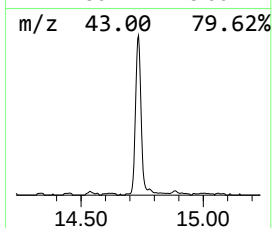
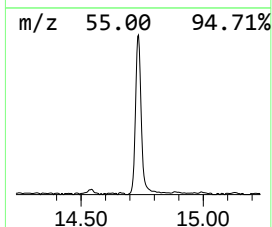
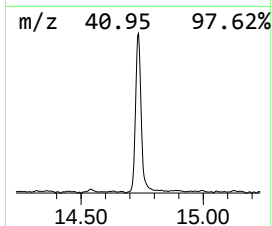
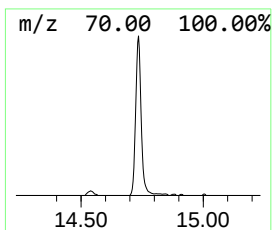
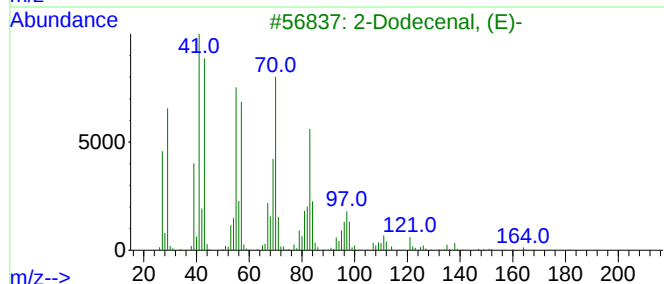
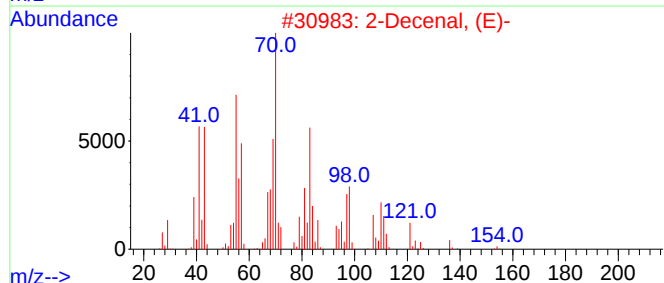
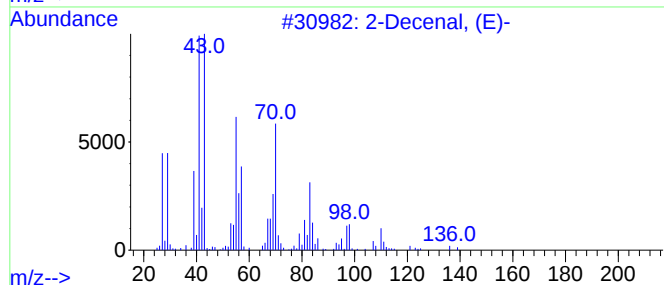
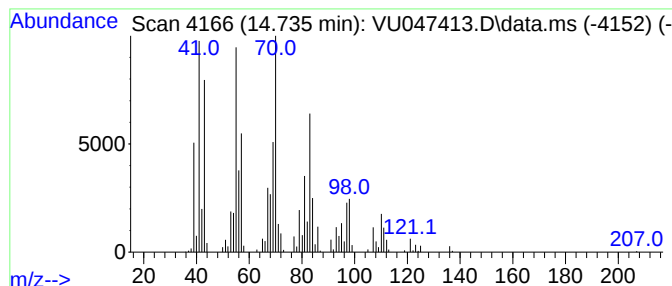
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 2-Decenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	2.98 ug/L	309763	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decenal, (E)-	154	C10H18O	003913-81-3	90
2			2-Decenal, (E)-	154	C10H18O	003913-81-3	90
3			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	64
4			2-Tridecenal, (E)-	196	C13H24O	007069-41-2	59
5			Cycloheptane	98	C7H14	000291-64-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU030922\
 Data File : VU047413.D
 Acq On : 09 Mar 2022 18:45
 Operator : SY/MD
 Sample : N1840-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFY22

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR030922WMA.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	2.1	ug/L	161799	1	6.253	379209	5.0
(DEL) Alkane: S...	2.211	1.0	ug/L	77164	1	6.253	379209	5.0
Pentanal	6.880	2.8	ug/L	214774	1	6.253	379209	5.0
Hexanal	8.787	17.9	ug/L	1665030	2	9.420	464479	5.0
Heptanal	10.343	6.6	ug/L	613992	2	9.420	464479	5.0
2-Heptenal, (E)-	11.295	0.6	ug/L	62833	3	11.812	519213	5.0
Octanal	11.687	9.1	ug/L	948434	3	11.812	519213	5.0
2-Dodecenal, (E)-	12.545	1.0	ug/L	104176	3	11.812	519213	5.0
Nonanal	12.886	15.4	ug/L	1596260	3	11.812	519213	5.0
2-Nonenal, (E)-	13.684	0.6	ug/L	63040	3	11.812	519213	5.0
2-Decenal, (E)-	14.735	3.0	ug/L	309763	3	11.812	519213	5.0