

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021622\
 Data File : VU047160.D
 Acq On : 16 Feb 2022 14:51
 Operator : SY/MD
 Sample : N1545-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXZ8

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: VU047160.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	25	rVB	278228	284323	11.08%	1.875%
2	1.494	41	48	68	rVB	46907	51064	1.99%	0.337%
3	1.604	71	82	95	rBV3	243230	316756	12.34%	2.089%
4	1.919	171	180	197	rVV	82501	116461	4.54%	0.768%
5	1.999	197	205	216	rVB	30546	42590	1.66%	0.281%
6	2.160	246	255	262	rBV2	21691	30257	1.18%	0.199%
7	2.208	262	270	281	rVB	94792	130938	5.10%	0.863%
8	2.571	367	383	401	rBV2	203430	397271	15.48%	2.619%
9	3.877	772	789	808	rBV2	21834	53405	2.08%	0.352%
10	4.459	953	970	988	rBV4	9050	26578	1.04%	0.175%
11	4.655	1014	1031	1084	rBV	88648	396549	15.45%	2.615%
12	5.070	1143	1160	1187	rBV2	145667	360357	14.04%	2.376%
13	5.729	1344	1365	1396	rBV2	296784	783318	30.52%	5.165%
14	6.253	1514	1528	1548	rBV	210029	402716	15.69%	2.655%
15	6.546	1603	1619	1634	rBV2	118950	227389	8.86%	1.499%
16	6.693	1651	1665	1687	rBV	180304	364424	14.20%	2.403%
17	6.883	1711	1724	1758	rBV	91922	196186	7.64%	1.294%
18	7.108	1783	1794	1807	rBV2	14933	28027	1.09%	0.185%
19	7.568	1923	1937	1962	rBV	105638	188754	7.35%	1.245%
20	7.902	2026	2041	2056	rBV	386271	693729	27.03%	4.574%
21	7.973	2057	2063	2084	rVB	16680	29758	1.16%	0.196%
22	8.182	2118	2128	2140	rBV	64566	106323	4.14%	0.701%
23	8.555	2231	2244	2257	rVV	80673	139622	5.44%	0.921%
24	8.639	2257	2270	2303	rVV	496454	984783	38.37%	6.493%
25	8.790	2303	2317	2364	rVB	1404815	2566846	100.00%	16.924%
26	9.420	2500	2513	2546	rVB	316630	542366	21.13%	3.576%
27	10.343	2790	2800	2827	rVB	238654	390928	15.23%	2.578%
28	10.758	2918	2929	2942	rBV	148315	236830	9.23%	1.562%
29	10.893	2958	2971	2985	rVB	24830	43207	1.68%	0.285%
30	11.295	3089	3096	3106	rVB	35752	55324	2.16%	0.365%
31	11.687	3206	3218	3233	rBV	481861	718489	27.99%	4.737%
32	11.812	3245	3257	3273	rVB	392450	626524	24.41%	4.131%
33	12.195	3359	3376	3396	rBV	384701	624568	24.33%	4.118%
34	12.545	3474	3485	3500	rBV	81835	135312	5.27%	0.892%
35	12.886	3578	3591	3616	rBV	1454580	2097405	81.71%	13.829%
36	13.687	3829	3840	3857	rBV4	34600	57843	2.25%	0.381%

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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\SFAMUTR021622WMA.M
Title : TRACE VOA SFAM1.0

37	14.735	4154	4166	4190	rBV	410469	617484	24.06%	4.071%
38	15.709	4458	4469	4491	rBV2	57779	101786	3.97%	0.671%

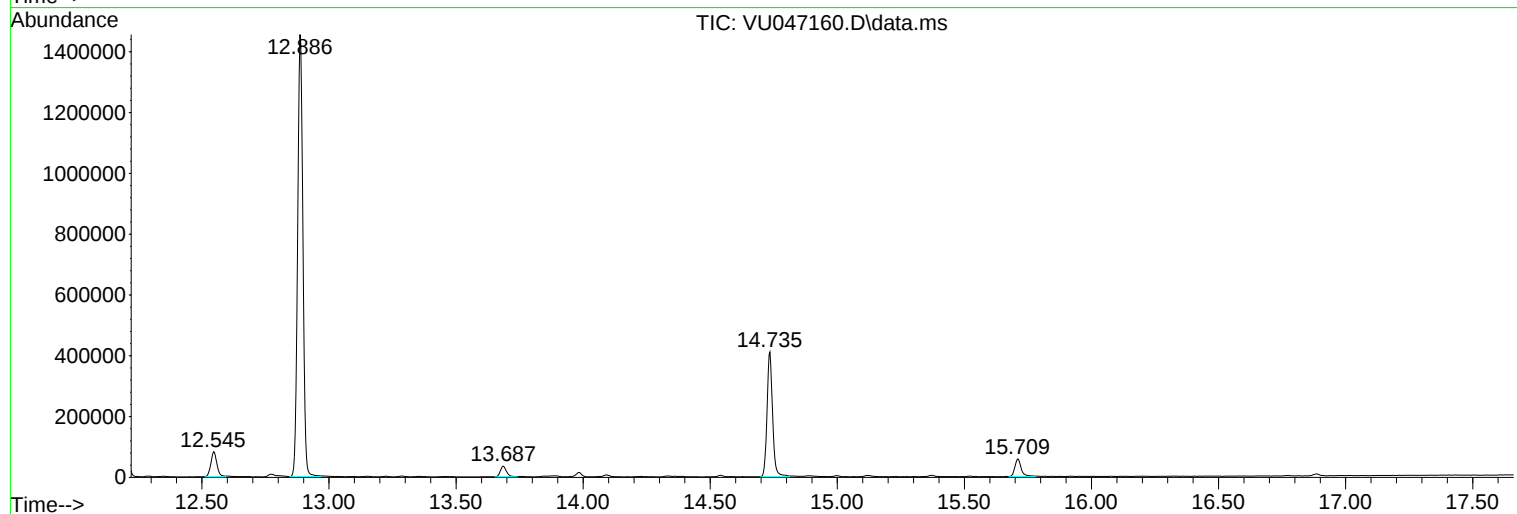
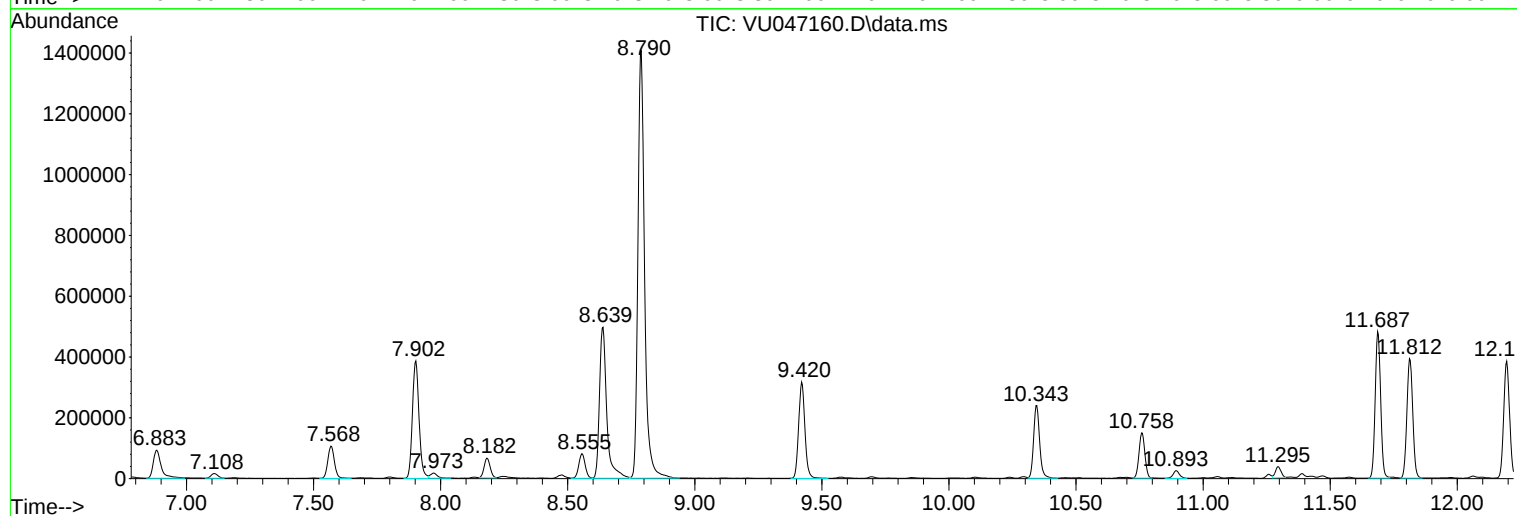
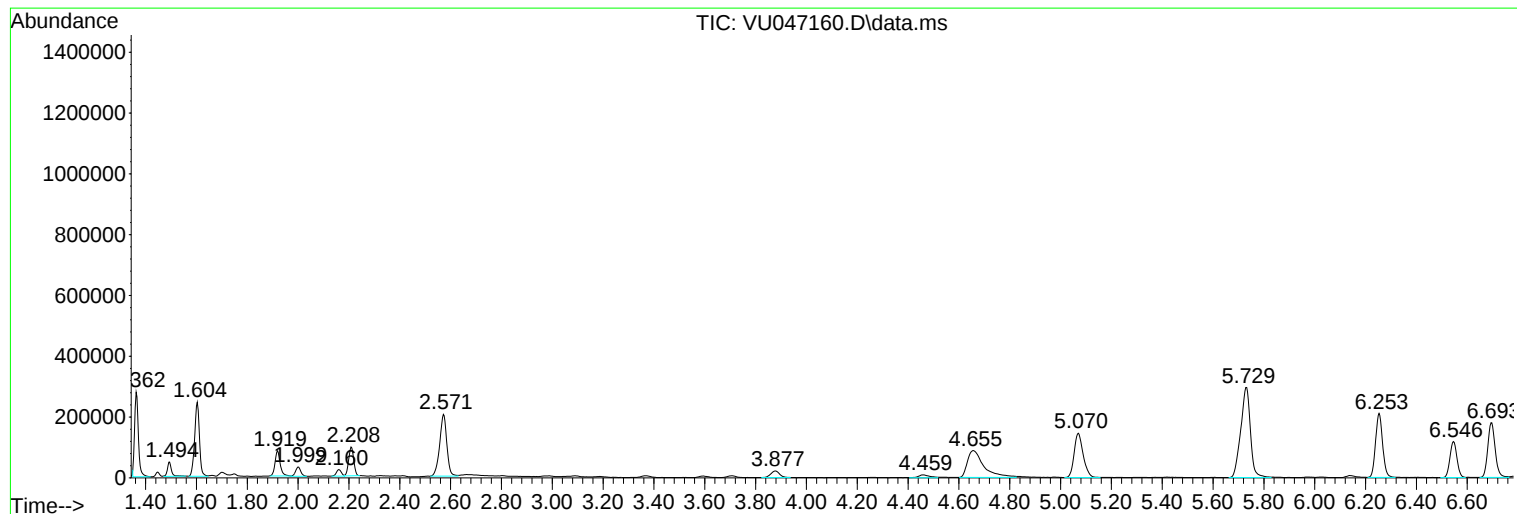
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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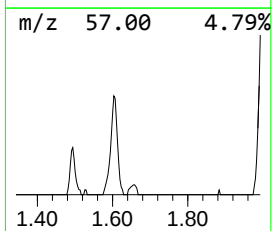
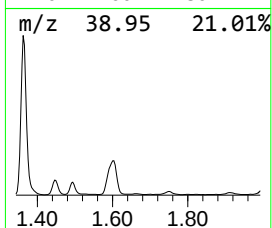
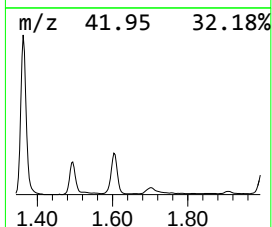
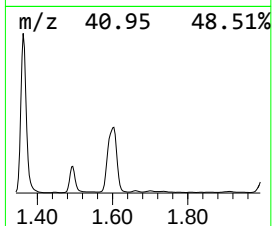
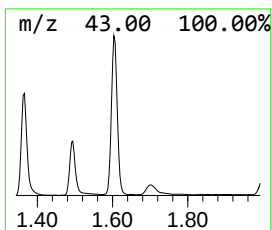
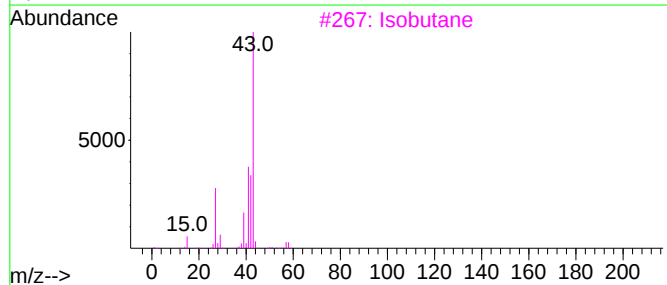
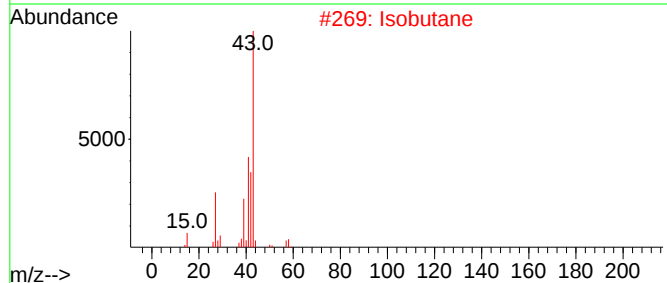
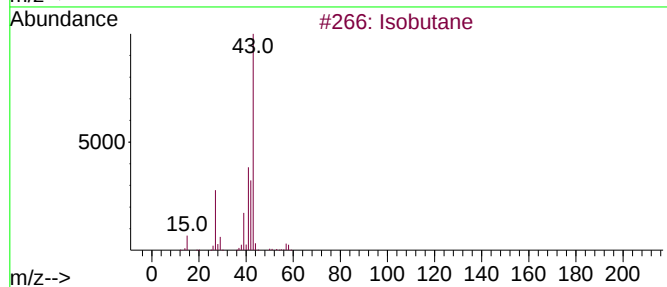
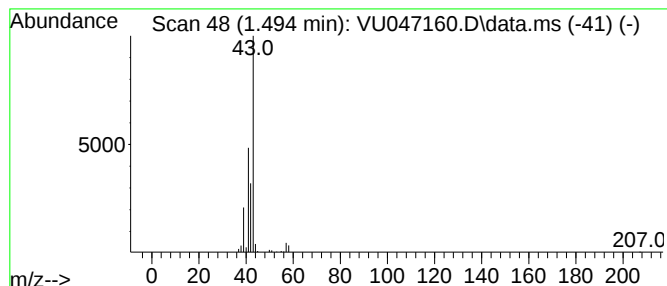
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.494	0.63 ug/L	51064	1,4-Difluorobenzene	6.253

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	80
2		Isobutane	58	C4H10	000075-28-5	64
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	64
5		Isobutane	58	C4H10	000075-28-5	45



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Instrument :
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ClientSampleId :
BFXZ8

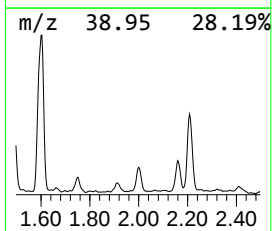
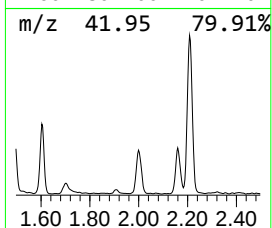
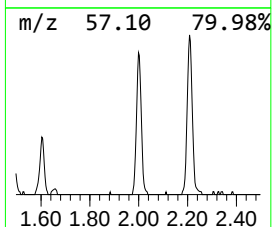
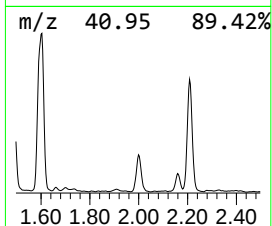
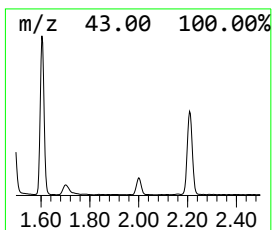
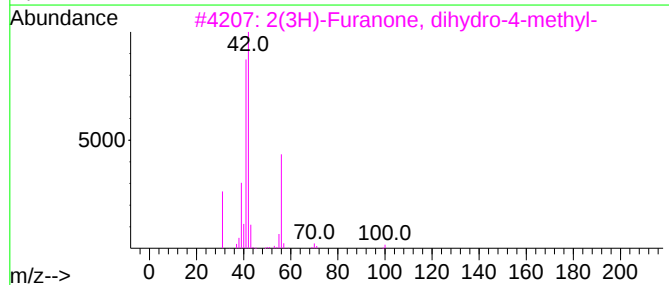
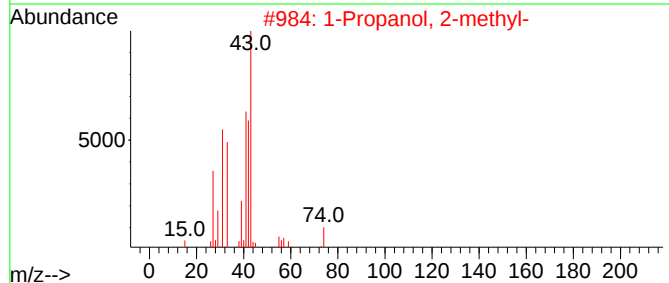
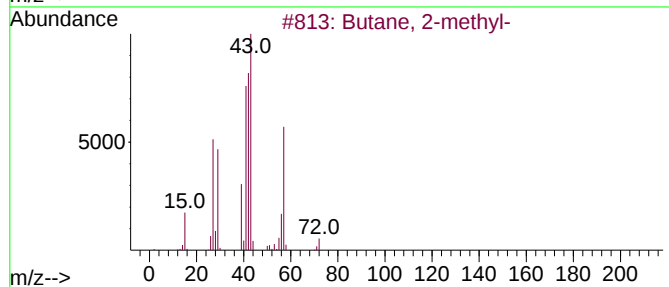
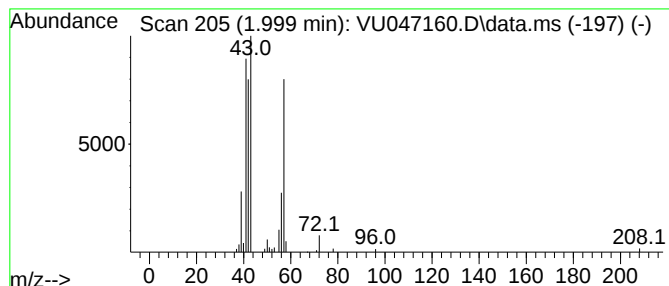
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.999	0.53 ug/L	42590	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	86
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	36
3			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	33
4			Pentane	72	C5H12	000109-66-0	33
5			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12



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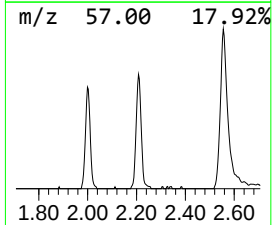
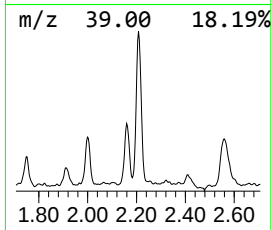
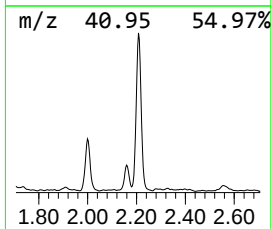
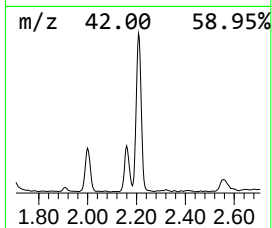
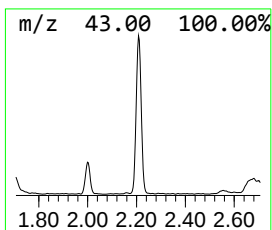
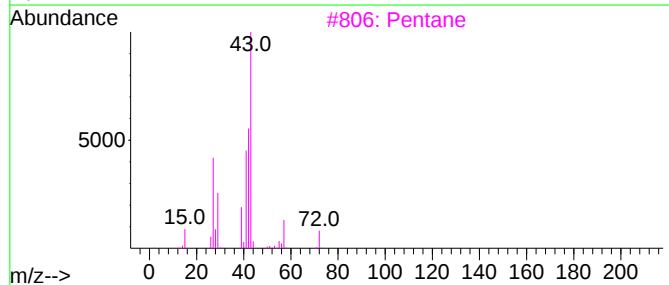
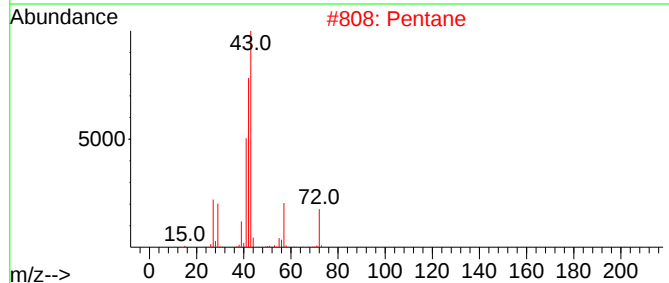
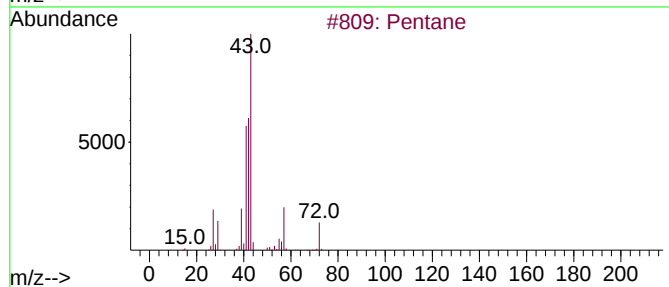
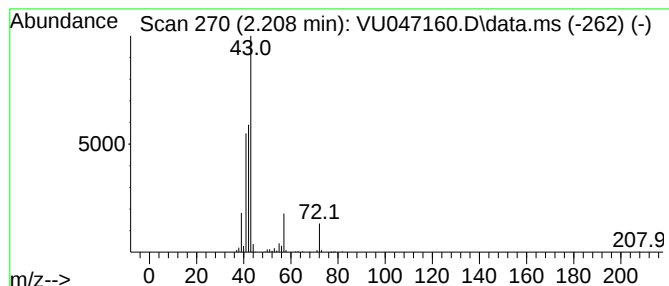
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.208	1.63 ug/L	130938	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	90
3	Pentane			72	C5H12	000109-66-0	86
4	Pentane			72	C5H12	000109-66-0	86
5	Pentane			72	C5H12	000109-66-0	86



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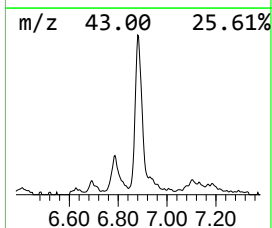
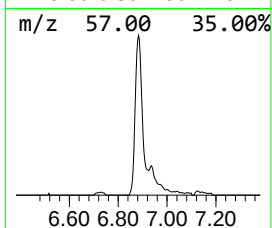
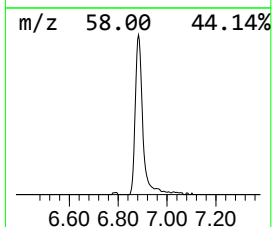
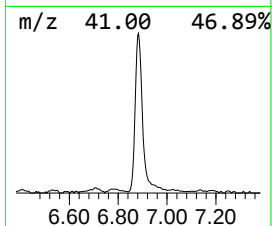
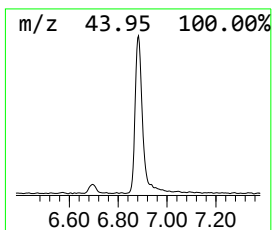
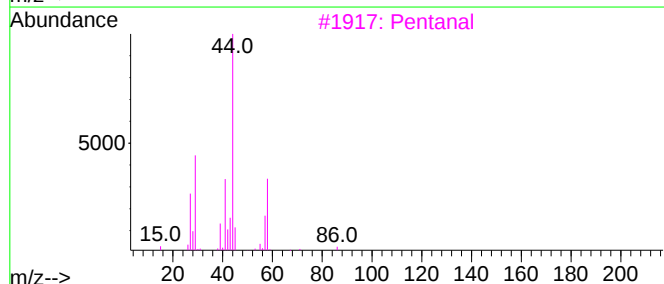
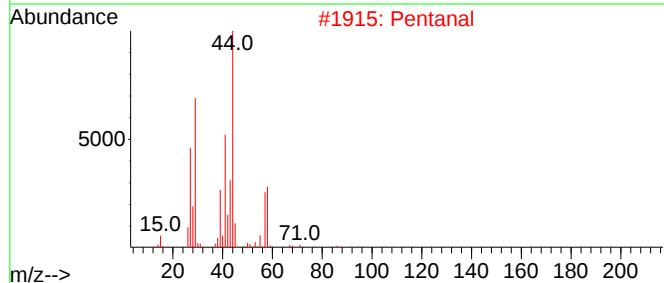
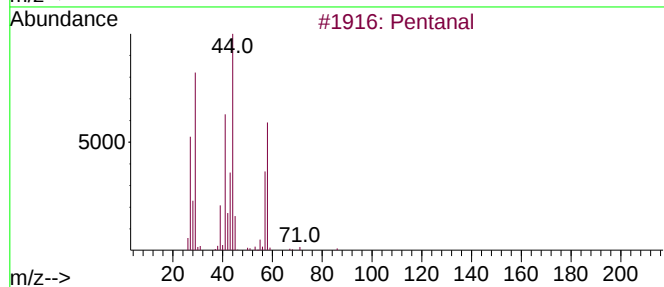
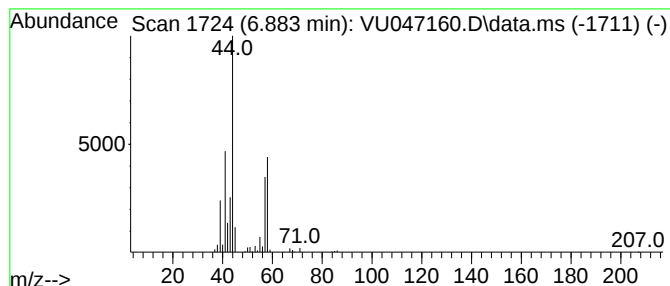
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Pentanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	2.44 ug/L	196186	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	Pentanal			86	C5H10O	000110-62-3	78
5	Butanal, 3-methyl-			86	C5H10O	000590-86-3	74



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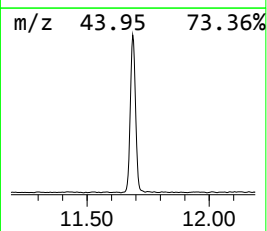
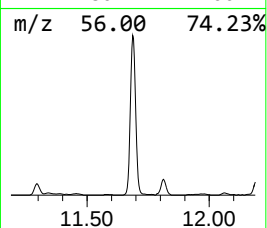
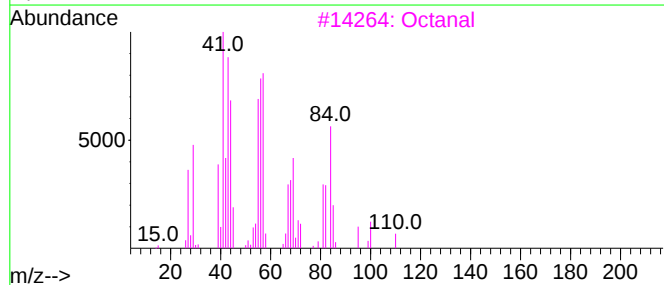
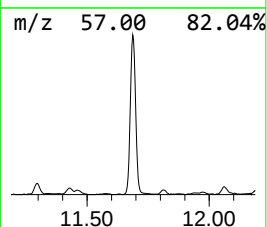
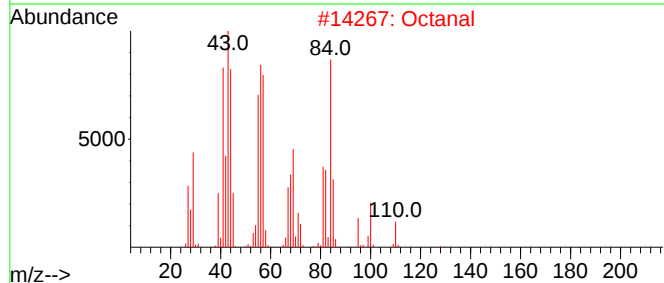
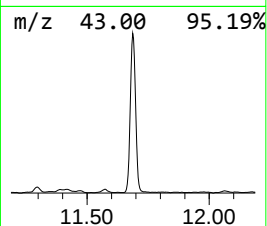
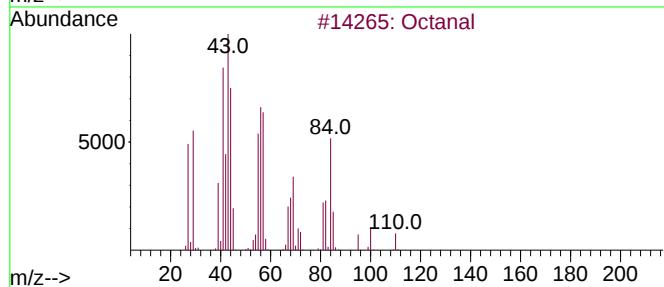
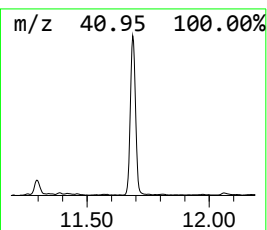
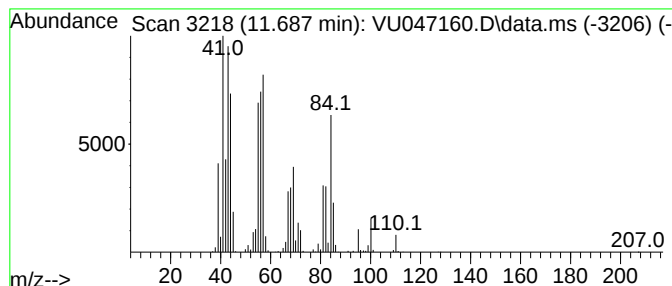
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	5.73 ug/L	718489	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	96
2	Octanal			128	C8H16O	000124-13-0	94
3	Octanal			128	C8H16O	000124-13-0	91
4	Octanal			128	C8H16O	000124-13-0	83
5	Octanal			128	C8H16O	000124-13-0	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021622\
Data File : VU047160.D
Acq On : 16 Feb 2022 14:51
Operator : SY/MD
Sample : N1545-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXZ8

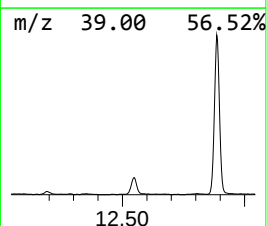
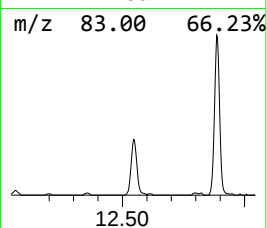
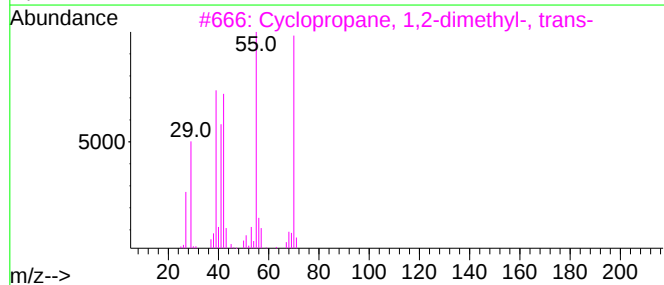
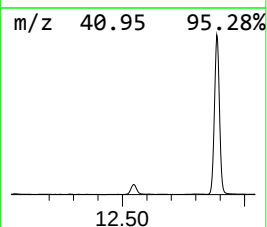
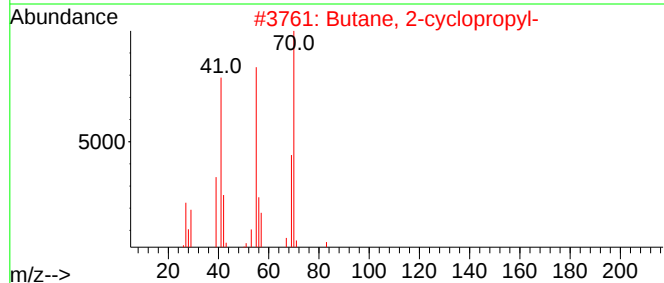
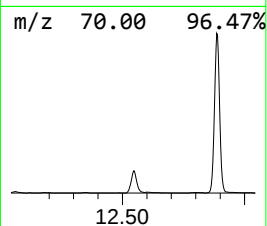
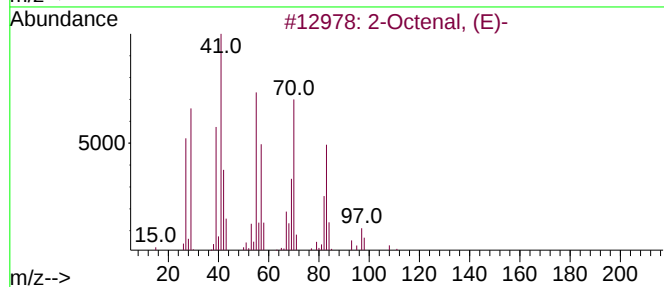
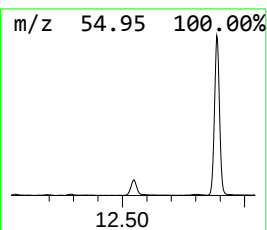
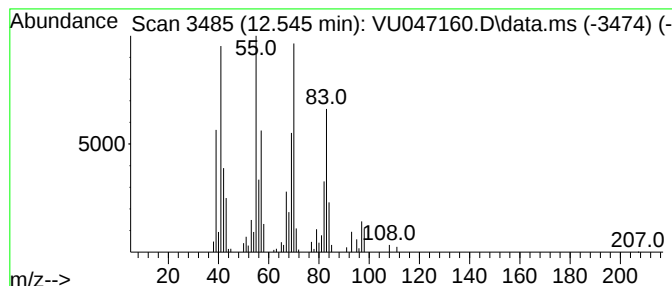
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 2-Octenal, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.545	1.08 ug/L	135312	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octenal, (E)-	126	C8H14O	002548-87-0	80
2			Butane, 2-cyclopropyl-	98	C7H14	005750-02-7	49
3			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	46
4			2-Pentene, (E)-	70	C5H10	000646-04-8	38
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021622\
Data File : VU047160.D
Acq On : 16 Feb 2022 14:51
Operator : SY/MD
Sample : N1545-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

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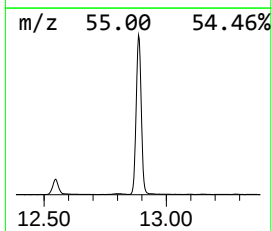
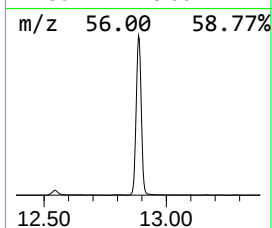
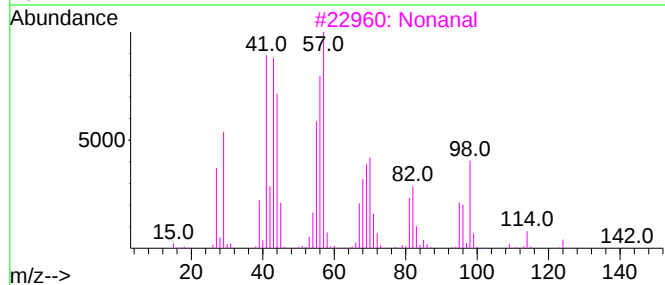
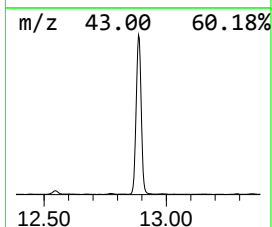
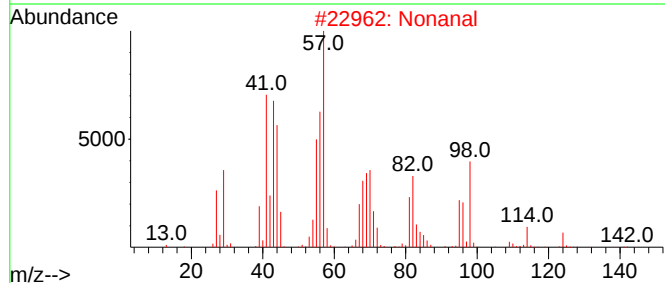
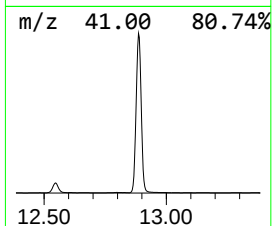
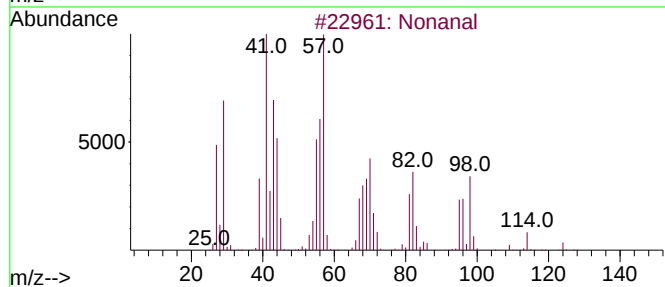
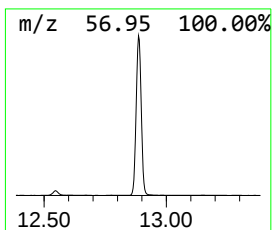
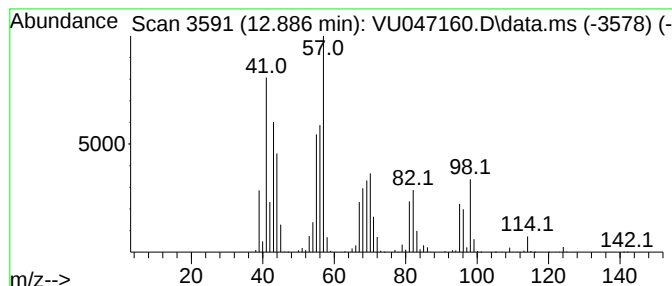
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	16.74 ug/L	2097410	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	90
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\VU021622\
Data File : VU047160.D
Acq On : 16 Feb 2022 14:51
Operator : SY/MD
Sample : N1545-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXZ8

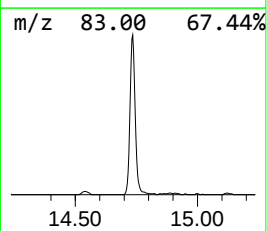
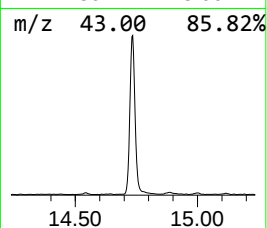
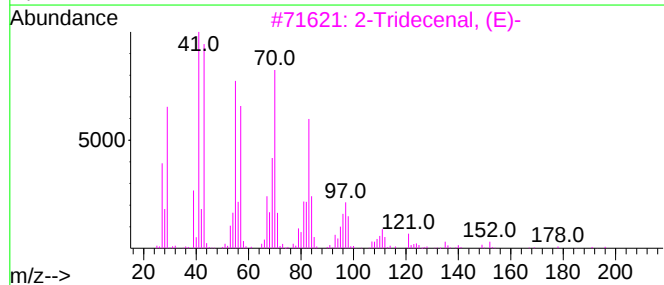
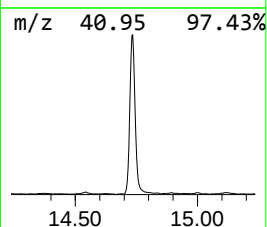
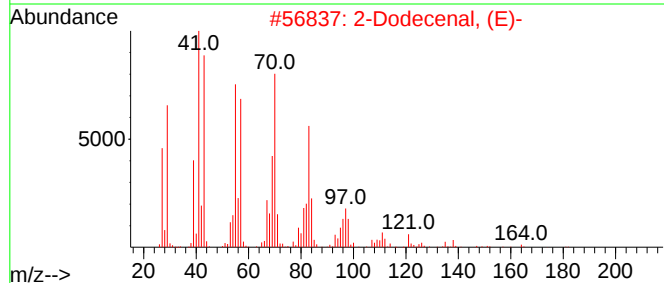
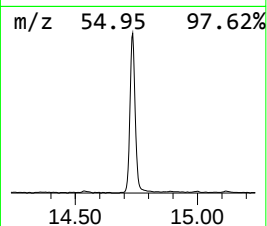
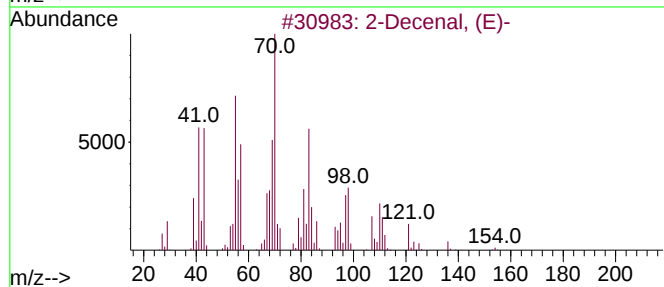
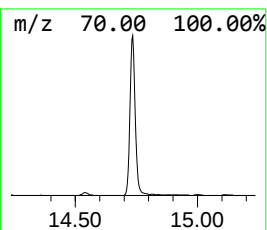
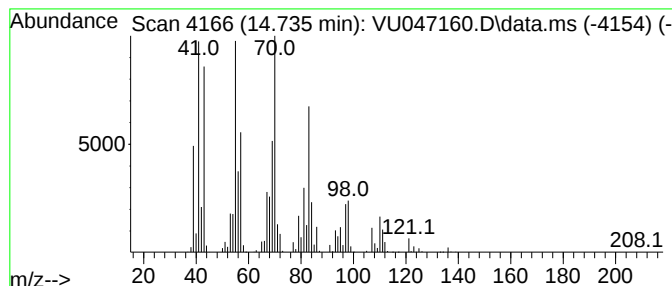
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 2-Decenal, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	4.93 ug/L	617484	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-Dodecenal, (E)-	182	C12H22O	020407-84-5	64
3			2-Tridecenal, (E)-	196	C13H24O	007069-41-2	59
4			2-Octenal, (E)-	126	C8H14O	002548-87-0	50
5			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021622\
Data File : VU047160.D
Acq On : 16 Feb 2022 14:51
Operator : SY/MD
Sample : N1545-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 11 Sample Multiplier: 1

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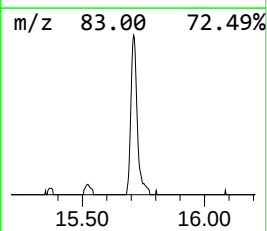
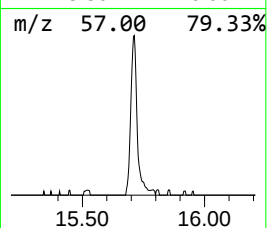
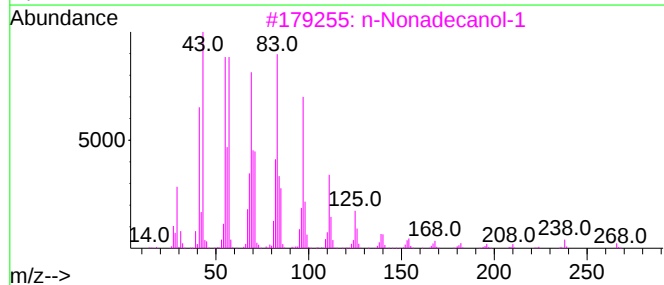
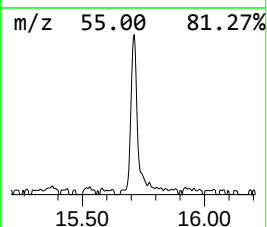
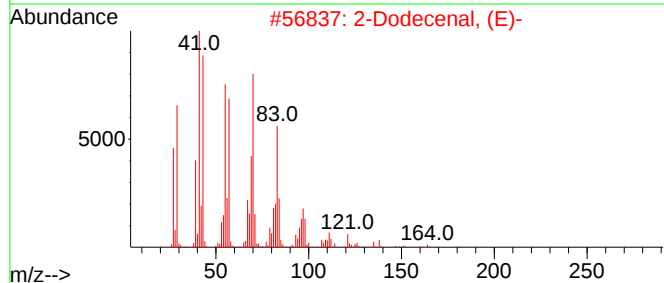
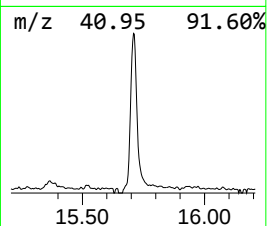
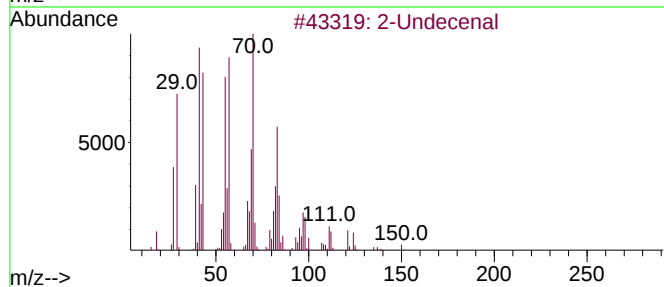
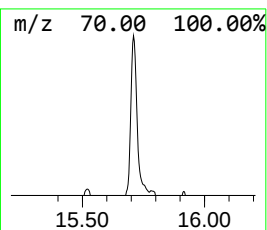
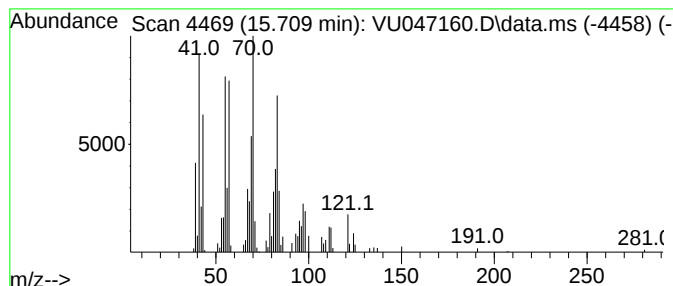
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2-Undecenal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.709	0.81 ug/L	101786	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Undecenal	168	C11H20O	002463-77-6	91
2			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	62
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	53
4			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	46
5			1,13-Tetradecadien-3-one	208	C14H24O	058879-40-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU021622\
 Data File : VU047160.D
 Acq On : 16 Feb 2022 14:51
 Operator : SY/MD
 Sample : N1545-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXZ8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR021622WMA.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...	1.494	0.6	ug/L	51064	1	6.253	402716	5.0
(DEL) Alkane: S...	1.999	0.5	ug/L	42590	1	6.253	402716	5.0
(DEL) Alkane: S...	2.208	1.6	ug/L	130938	1	6.253	402716	5.0
Pentanal	6.883	2.4	ug/L	196186	1	6.253	402716	5.0
Octanal	11.687	5.7	ug/L	718489	3	11.812	626524	5.0
2-Octenal, (E)-	12.545	1.1	ug/L	135312	3	11.812	626524	5.0
Nonanal	12.886	16.7	ug/L	2097410	3	11.812	626524	5.0
2-Decenal, (E)-	14.735	4.9	ug/L	617484	3	11.812	626524	5.0
2-Undecenal	15.709	0.8	ug/L	101786	3	11.812	626524	5.0