

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
 Data File : VU046739.D
 Acq On : 12 Jan 2022 13:52
 Operator : SY/MD
 Sample : N1101-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFXW7

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\SFAMUTR122121WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU046739.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	72	81	90	rBV	30673	40060	2.32%	0.664%
2	1.919	172	180	197	rVB	23850	32077	1.86%	0.531%
3	2.578	366	385	400	rBV3	69441	140948	8.17%	2.335%
4	4.646	1007	1028	1068	rBV2	40301	155957	9.04%	2.584%
5	5.067	1144	1159	1179	rVB	50814	115074	6.67%	1.907%
6	5.321	1221	1238	1254	rVB	31864	69815	4.05%	1.157%
7	5.729	1344	1365	1388	rBV2	95792	253091	14.67%	4.193%
8	6.250	1513	1527	1549	rBV	95358	177212	10.27%	2.936%
9	6.546	1608	1619	1630	rBV3	10133	18650	1.08%	0.309%
10	6.694	1652	1665	1681	rBV	61456	120837	7.01%	2.002%
11	6.880	1711	1723	1741	rBV2	20424	40556	2.35%	0.672%
12	7.568	1926	1937	1955	rBV2	31291	55508	3.22%	0.920%
13	7.900	2027	2040	2054	rBV	112725	194288	11.26%	3.219%
14	8.183	2117	2128	2141	rBV	19804	33333	1.93%	0.552%
15	8.556	2231	2244	2257	rBV	248185	422064	24.47%	6.993%
16	8.636	2257	2269	2300	rVV	209647	388917	22.55%	6.444%
17	8.787	2303	2316	2350	rVB	164443	282055	16.35%	4.673%
18	9.417	2500	2512	2529	rBV	141886	235500	13.65%	3.902%
19	10.343	2789	2800	2825	rBV	80728	129811	7.53%	2.151%
20	10.758	2917	2929	2945	rVB	66963	103999	6.03%	1.723%
21	11.687	3205	3218	3233	rBV	422804	619903	35.94%	10.271%
22	11.813	3244	3257	3272	rVB	182972	287749	16.68%	4.768%
23	12.192	3364	3375	3390	rVB	135786	215562	12.50%	3.572%
24	12.543	3471	3484	3499	rBV3	28219	55155	3.20%	0.914%
25	12.887	3577	3591	3622	rBV	1193696	1724980	100.00%	28.581%
26	14.652	4132	4140	4156	rBV3	12459	22909	1.33%	0.380%
27	14.732	4156	4165	4176	rVV2	40771	62462	3.62%	1.035%
28	16.883	4822	4834	4851	rVB4	21727	37012	2.15%	0.613%

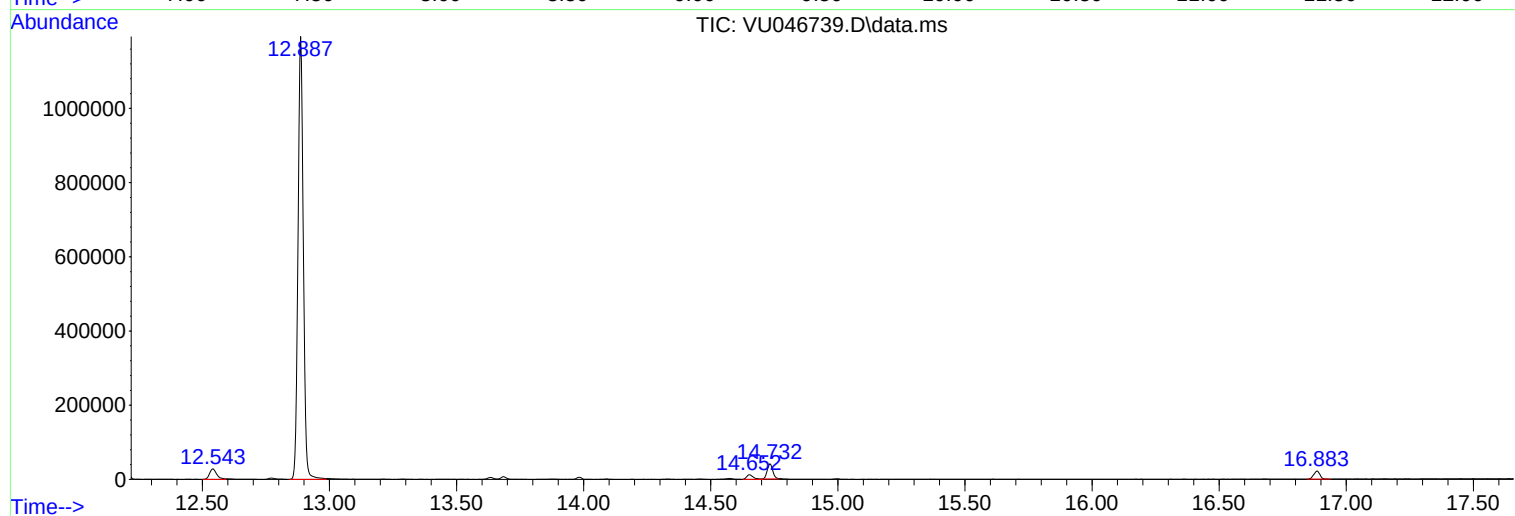
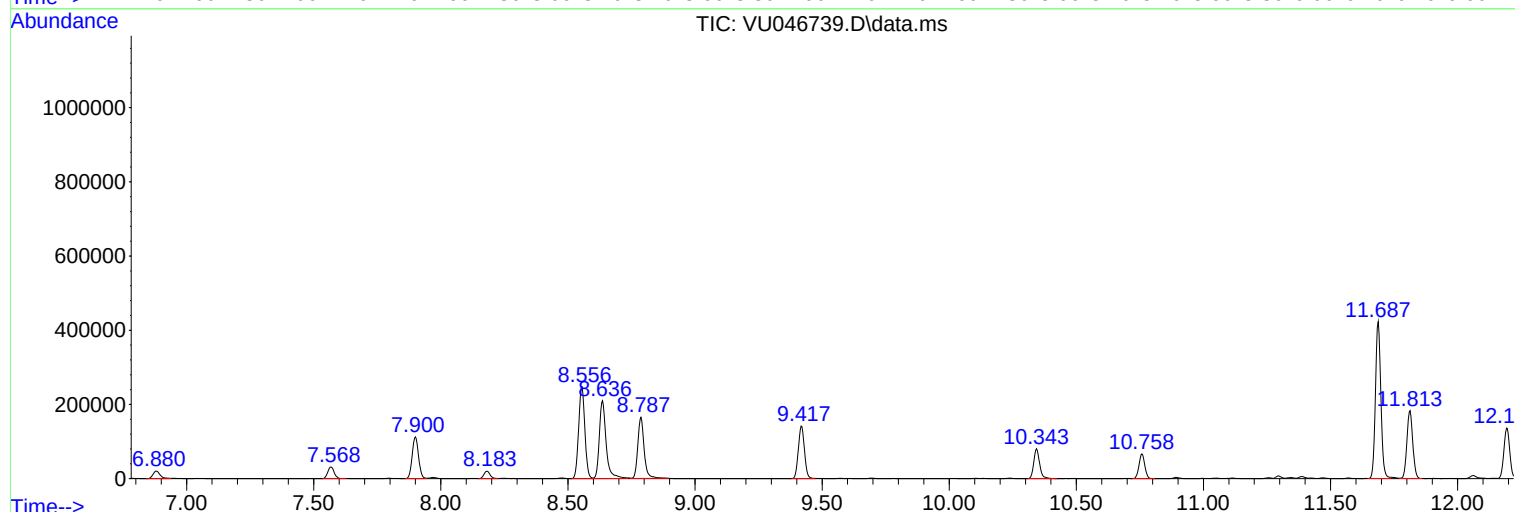
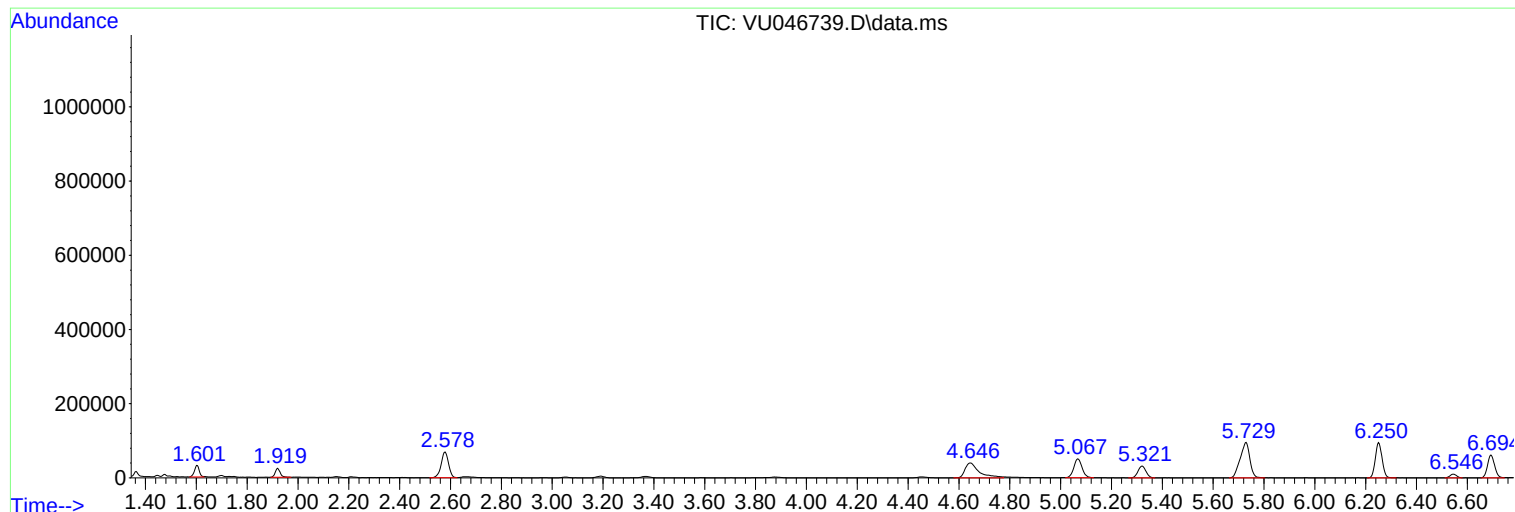
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ClientSampleId :
BFXW7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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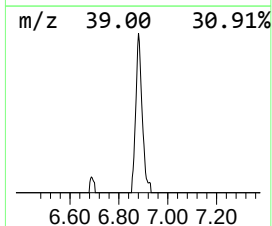
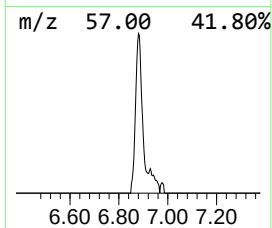
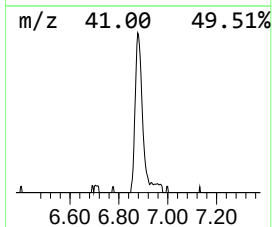
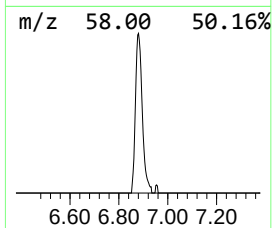
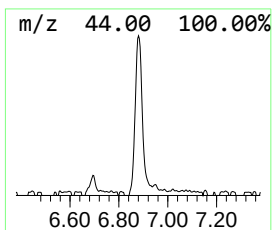
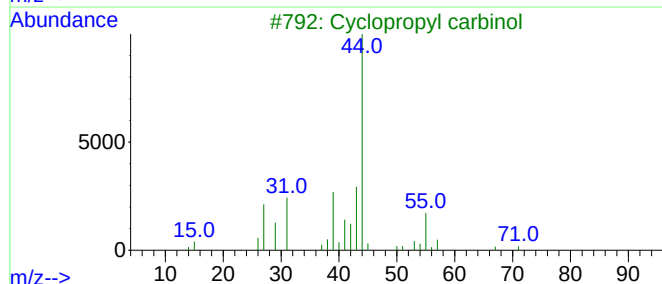
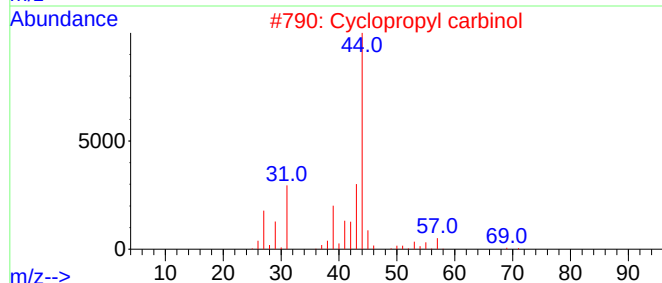
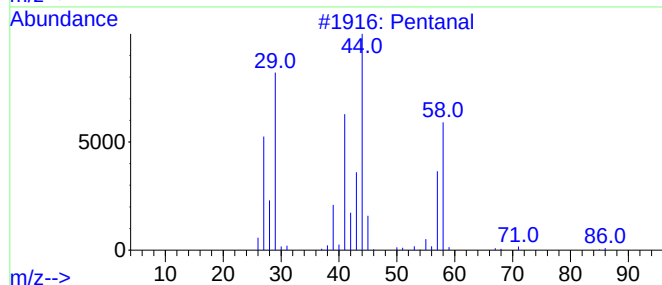
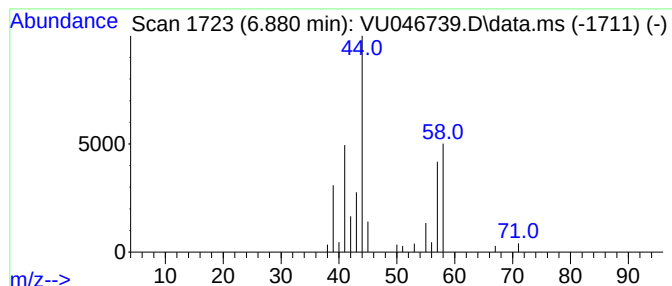
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	1.14 ug/L	40556	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	56
2			Cyclopropyl carbinol	72	C4H8O	002516-33-8	28
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	9
4			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	9
5			Pentanal	86	C5H10O	000110-62-3	9



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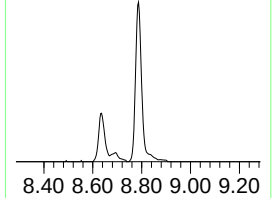
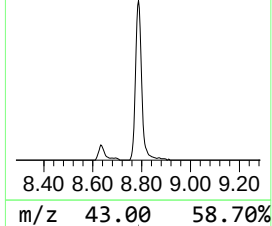
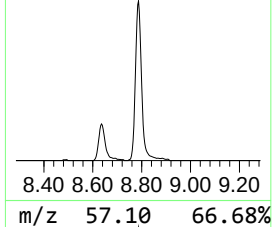
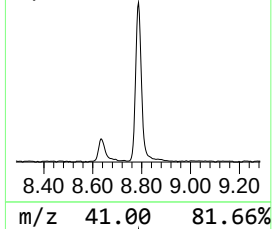
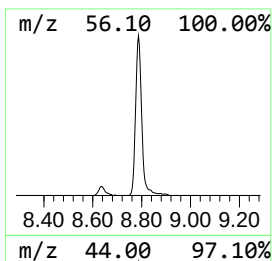
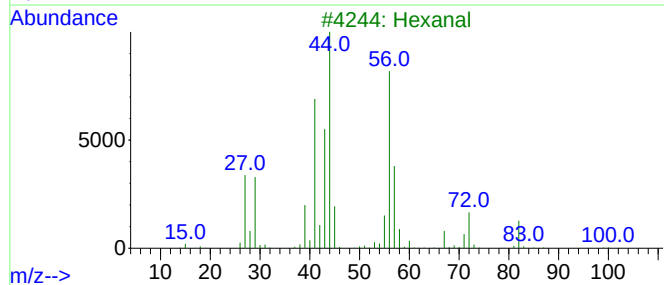
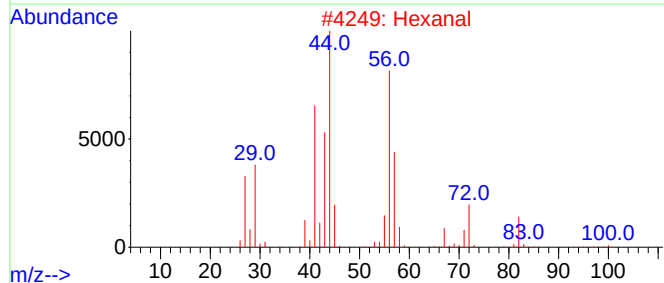
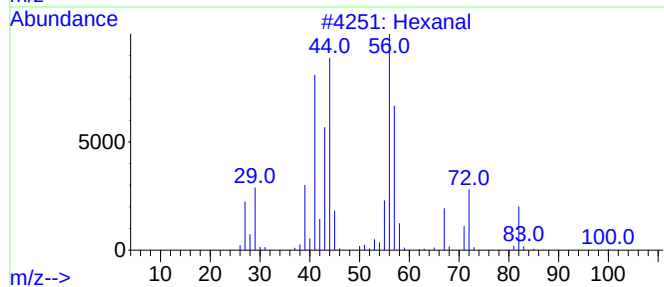
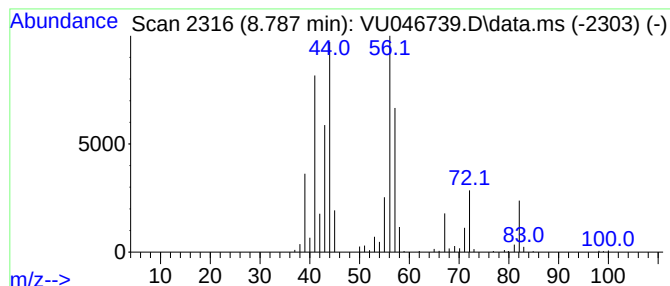
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	5.99 ug/L	282055	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	96
2	Hexanal			100	C6H12O	000066-25-1	91
3	Hexanal			100	C6H12O	000066-25-1	91
4	Hexanal			100	C6H12O	000066-25-1	90
5	Hexanal			100	C6H12O	000066-25-1	64



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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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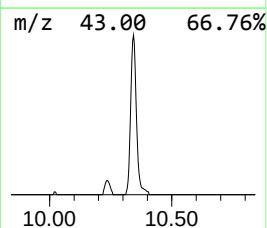
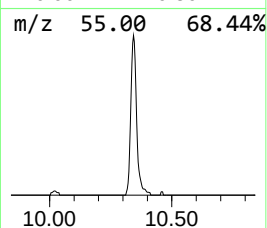
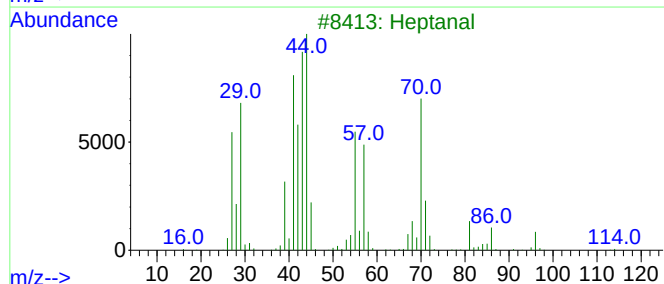
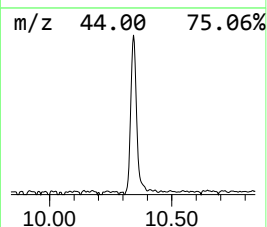
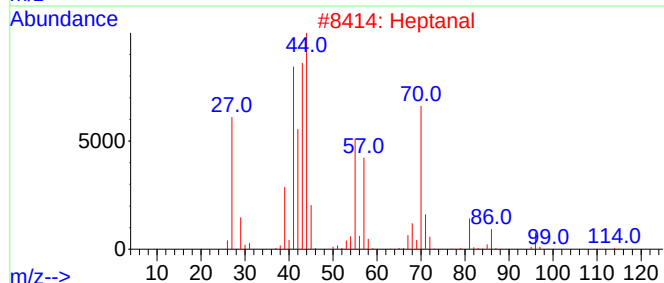
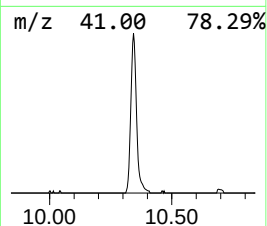
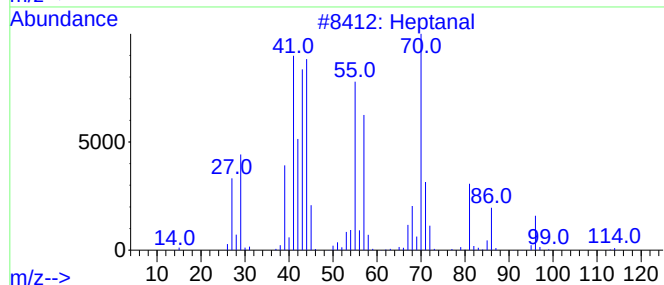
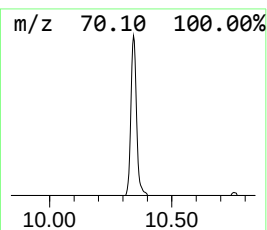
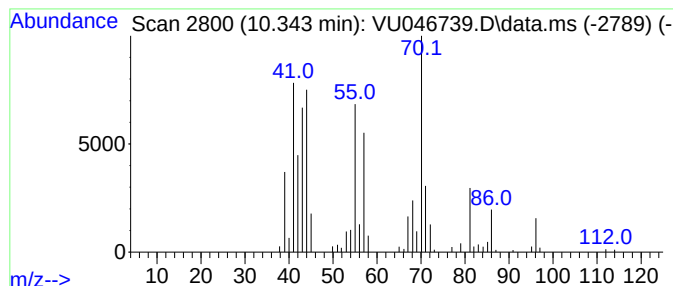
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.343	2.76 ug/L	129811	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	96
2			Heptanal	114	C7H14O	000111-71-7	95
3			Heptanal	114	C7H14O	000111-71-7	95
4			Heptanal	114	C7H14O	000111-71-7	90
5			Hexanal, 3-methyl-	114	C7H14O	019269-28-4	47



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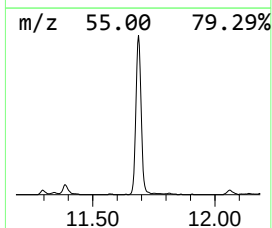
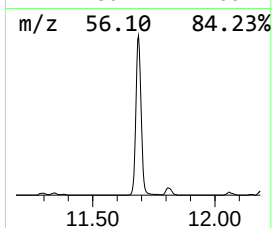
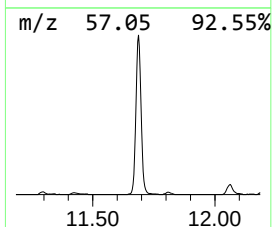
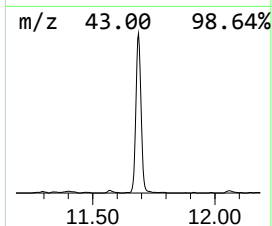
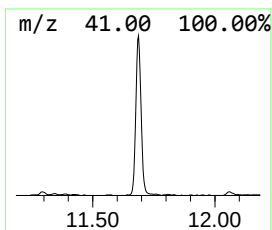
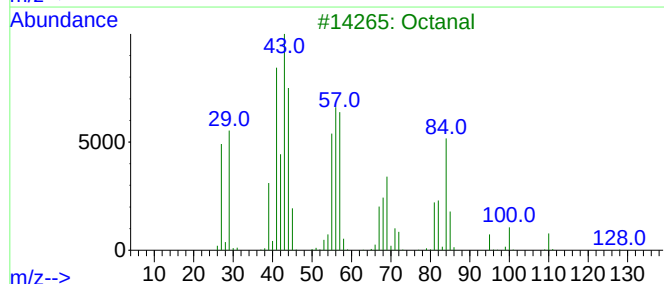
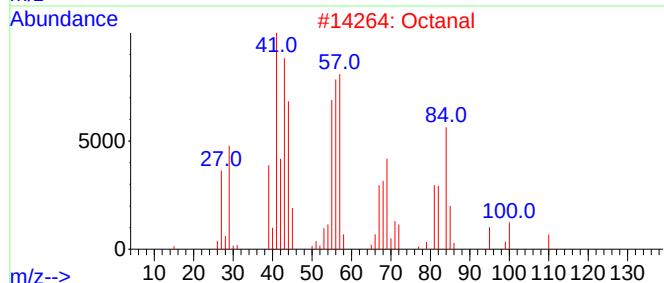
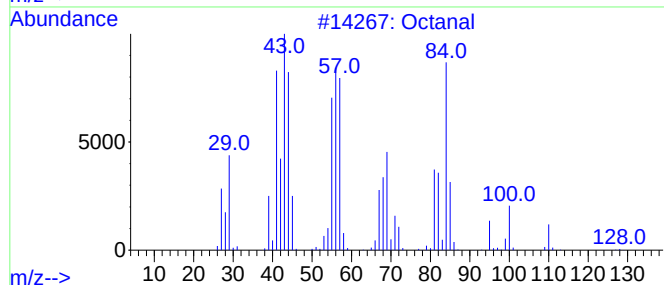
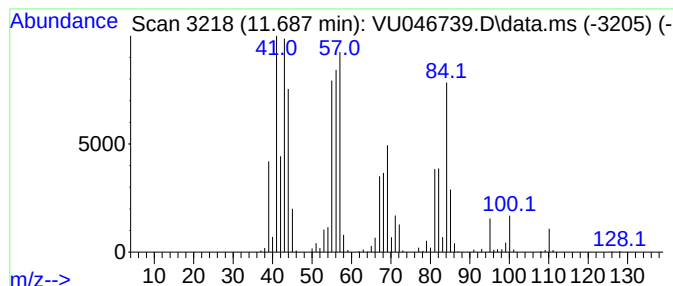
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	10.77 ug/L	619903	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal			128	C8H16O	000124-13-0	98
2	Octanal			128	C8H16O	000124-13-0	91
3	Octanal			128	C8H16O	000124-13-0	64
4	Octanal			128	C8H16O	000124-13-0	52
5	Cyclopentanol, 2-methyl-, cis-			100	C6H12O	025144-05-2	46



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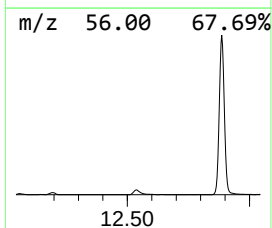
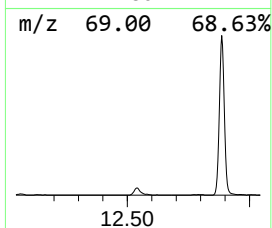
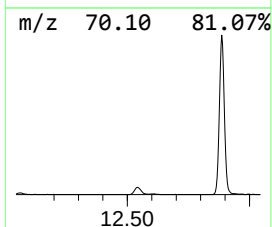
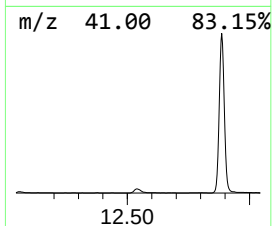
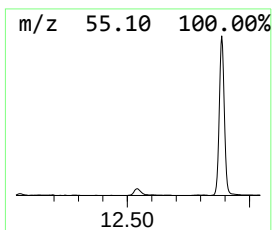
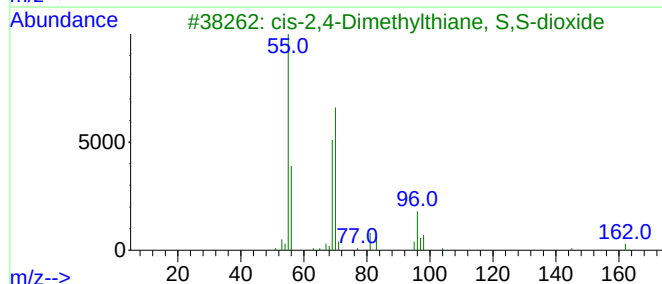
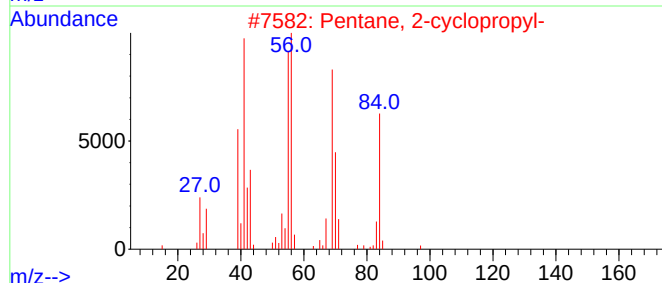
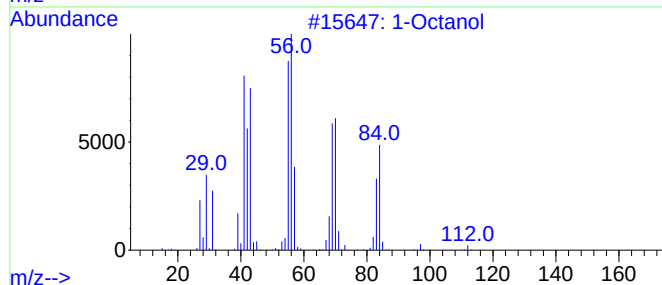
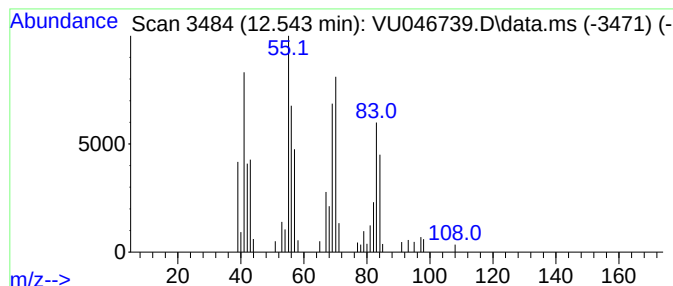
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.543	0.96 ug/L	55155	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	43
2			Pentane, 2-cyclopropyl-	112	C8H16	005458-16-2	38
3			cis-2,4-Dimethylthiane, S,S-dioxide	162	C7H14O2S	1000215-67-5	38
4			3-Hexene, (Z)-	84	C6H12	007642-09-3	35
5			2-Hexene, (Z)-	84	C6H12	007688-21-3	35



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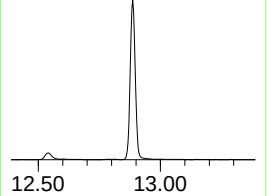
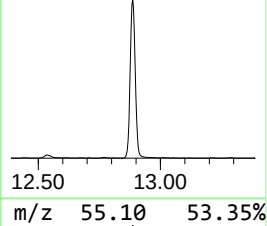
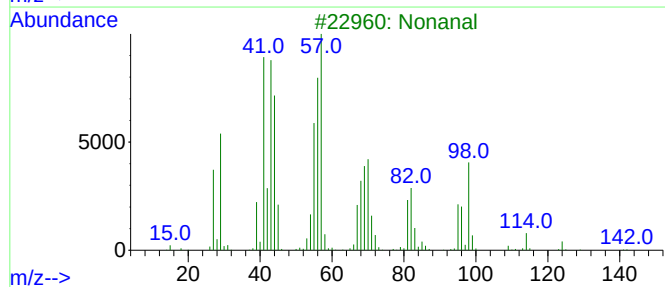
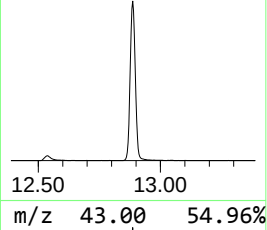
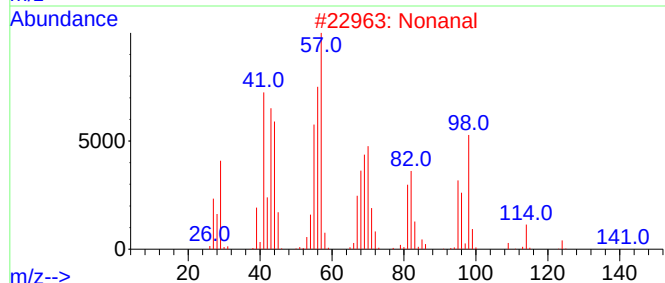
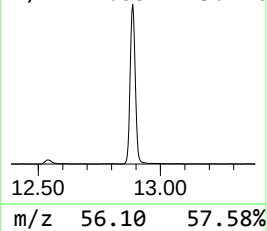
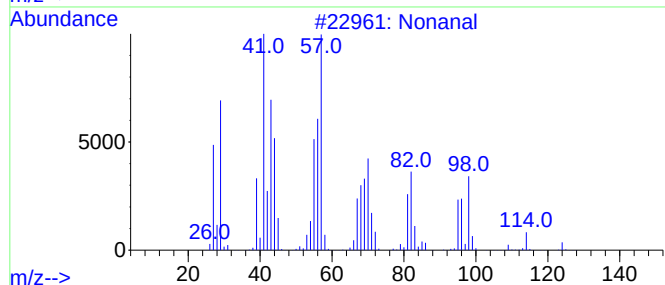
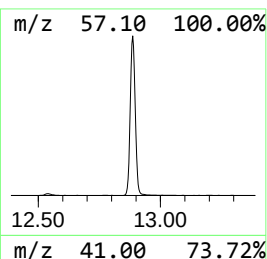
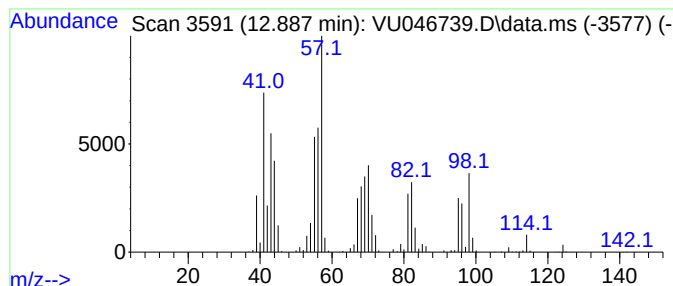
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.887	29.97 ug/L	1724980	1,4-Dichlorobenzene-d4	11.813

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	83
4			Nonanal	142	C9H18O	000124-19-6	72
5			Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046739.D
Acq On : 12 Jan 2022 13:52
Operator : SY/MD
Sample : N1101-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW7

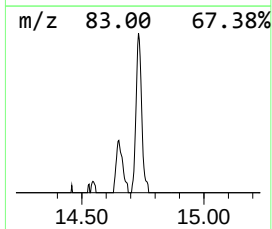
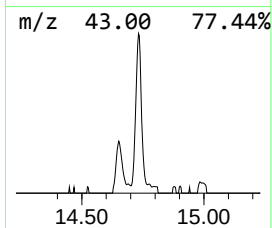
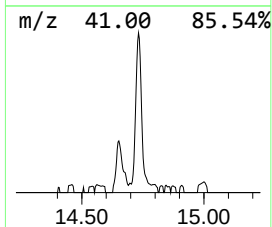
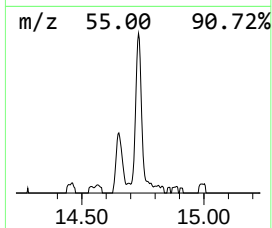
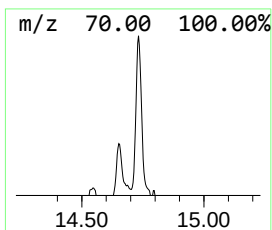
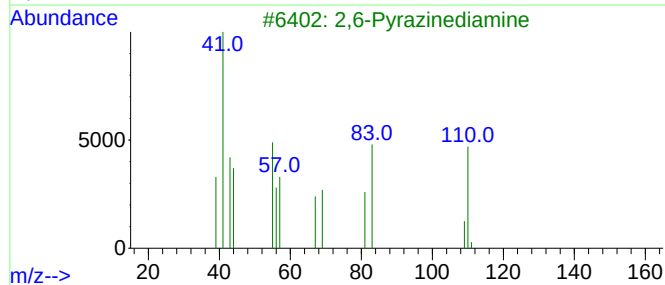
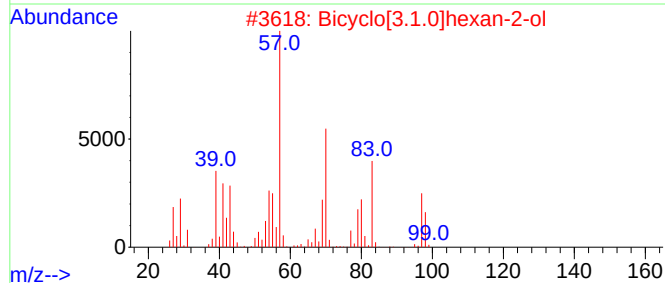
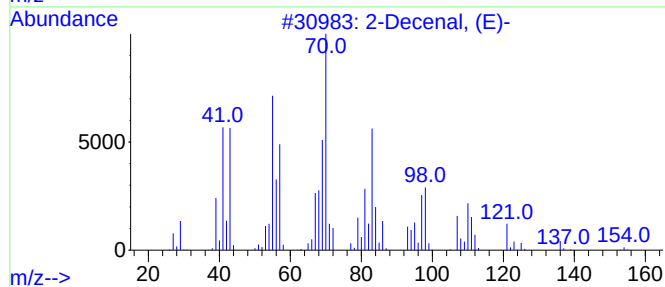
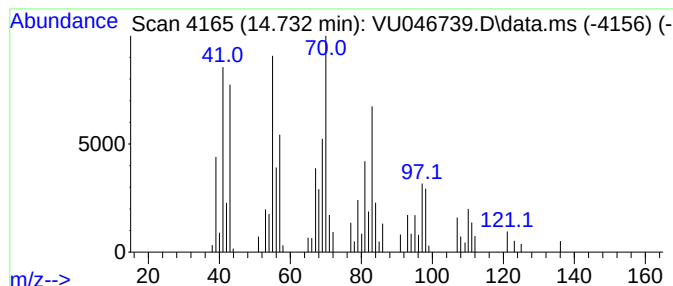
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 2-Decenal, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.732	1.09 ug/L	62462	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Decenal, (E)-	154	C10H18O	003913-81-3	58
2			Bicyclo[3.1.0]hexan-2-ol	98	C6H10O	1000194-18-6	49
3			2,6-Pyrazinediamine	110	C4H6N4	041536-80-5	46
4			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	46
5			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046739.D
Acq On : 12 Jan 2022 13:52
Operator : SY/MD
Sample : N1101-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW7

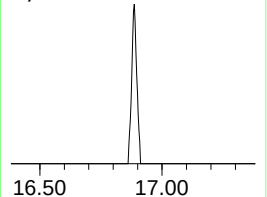
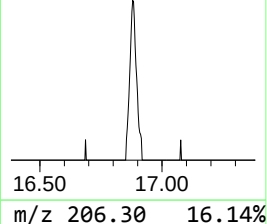
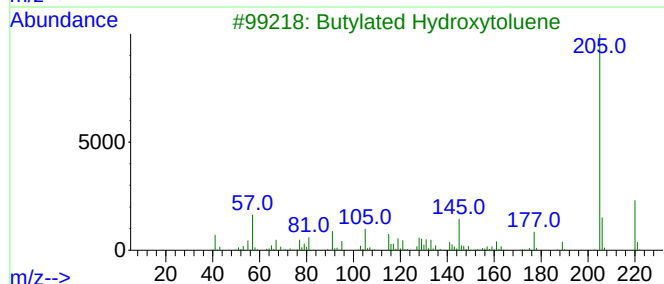
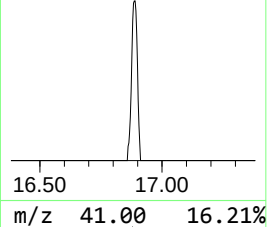
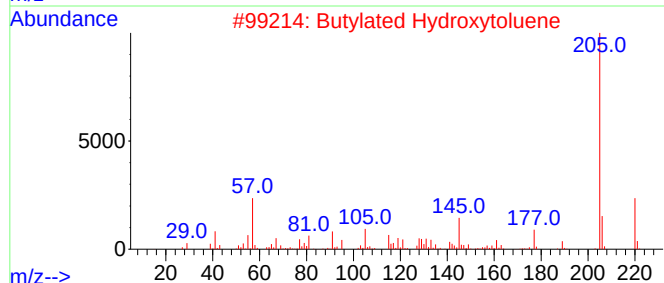
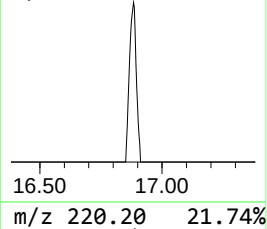
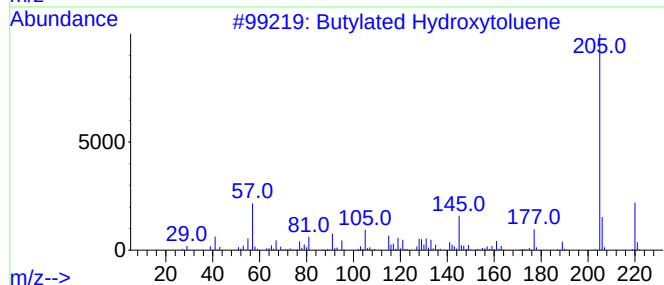
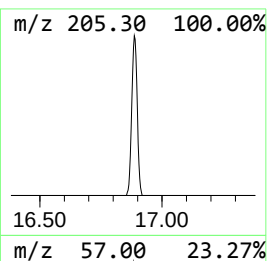
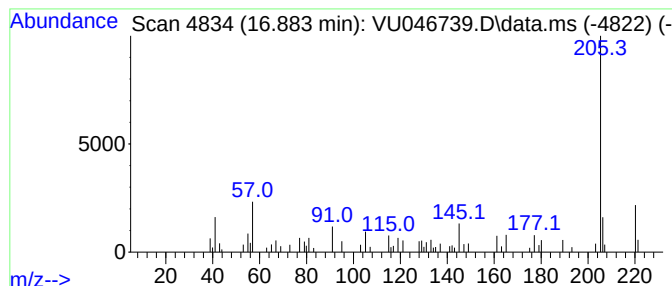
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Butylated Hydroxytoluene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	0.64 ug/L	37012	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
4			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	95
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011222\
Data File : VU046739.D
Acq On : 12 Jan 2022 13:52
Operator : SY/MD
Sample : N1101-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXW7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	6.880	1.1	ug/L	40556	1	6.250	177212	5.0
Hexanal	8.787	6.0	ug/L	282055	2	9.420	235500	5.0
Heptanal	10.343	2.8	ug/L	129811	2	9.420	235500	5.0
Octanal	11.687	10.8	ug/L	619903	3	11.813	287749	5.0
unknown-01	12.543	1.0	ug/L	55155	3	11.813	287749	5.0
Nonanal	12.887	30.0	ug/L	1724980	3	11.813	287749	5.0
2-Decenal, (E)-	14.732	1.1	ug/L	62462	3	11.813	287749	5.0
Butylated Hydro...	16.883	0.6	ug/L	37012	3	11.813	287749	5.0