

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032122\
 Data File : VV025114.D
 Acq On : 21 Mar 2022 13:14
 Operator : SY/MD
 Sample : N2044-04
 Misc : 25mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFY28

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_V\Method\SFAMVTR031522WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV025114.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.111	16	22	36	rVB	25478	24947	3.29%	0.402%
2	1.179	37	43	50	rBV	17912	17147	2.26%	0.276%
3	1.307	73	83	95	rVB	87165	97394	12.83%	1.568%
4	1.568	156	164	176	rBV	63173	71989	9.49%	1.159%
5	1.806	232	238	253	rVB	17583	24337	3.21%	0.392%
6	2.108	320	332	350	rBV2	135542	211046	27.81%	3.398%
7	3.912	882	893	930	rBV2	27124	116234	15.32%	1.871%
8	4.352	1015	1030	1056	rBV	81399	209597	27.62%	3.374%
9	5.050	1232	1247	1275	rBV3	192489	476154	62.75%	7.666%
10	5.619	1412	1424	1453	rBV	161235	328064	43.23%	5.282%
11	5.918	1507	1517	1533	rVB7	3987	10117	1.33%	0.163%
12	6.072	1551	1565	1592	rBV	103488	215482	28.40%	3.469%
13	6.291	1623	1633	1662	rBV2	31337	71764	9.46%	1.155%
14	6.989	1840	1850	1875	rBV	45793	86508	11.40%	1.393%
15	7.317	1938	1952	1970	rBV	230184	403125	53.12%	6.490%
16	7.400	1970	1978	1992	rVB	7861	15094	1.99%	0.243%
17	7.625	2039	2048	2069	rBV	24345	44114	5.81%	0.710%
18	7.940	2132	2146	2156	rBV3	4606	8624	1.14%	0.139%
19	8.092	2182	2193	2227	rBV	168837	345367	45.51%	5.560%
20	8.236	2227	2238	2273	rVV	453705	758858	100.00%	12.217%
21	8.850	2419	2429	2462	rBV	226714	374081	49.30%	6.023%
22	9.146	2512	2521	2538	rVB3	4684	7935	1.05%	0.128%
23	9.805	2717	2726	2749	rBV	84316	138783	18.29%	2.234%
24	10.217	2842	2854	2869	rBV	63973	101232	13.34%	1.630%
25	10.381	2891	2905	2916	rVB3	10334	16773	2.21%	0.270%
26	10.719	3001	3010	3015	rBV	10431	13932	1.84%	0.224%
27	10.757	3015	3022	3039	rVB2	27929	46159	6.08%	0.743%
28	10.857	3046	3053	3061	rBV2	9589	14564	1.92%	0.234%
29	10.911	3063	3070	3090	rVB10	5319	13680	1.80%	0.220%
30	11.146	3133	3143	3164	rBV	255520	385208	50.76%	6.202%
31	11.246	3164	3174	3196	rVB	221322	340660	44.89%	5.484%
32	11.622	3280	3291	3308	rVB	185092	285526	37.63%	4.597%
33	12.008	3402	3411	3426	rBV2	24657	45356	5.98%	0.730%
34	12.249	3475	3486	3498	rBV2	7870	12255	1.61%	0.197%
35	12.342	3502	3515	3537	rBV	297288	444751	58.61%	7.160%
36	13.136	3753	3762	3780	rBV5	13196	21075	2.78%	0.339%

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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

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37	14.037	4032	4042	4054	rVB2	6882	11196	1.48%	0.180%
38	14.175	4072	4085	4111	rBV	208110	355209	46.81%	5.719%
39	15.143	4378	4386	4405	rVB2	30196	47001	6.19%	0.757%

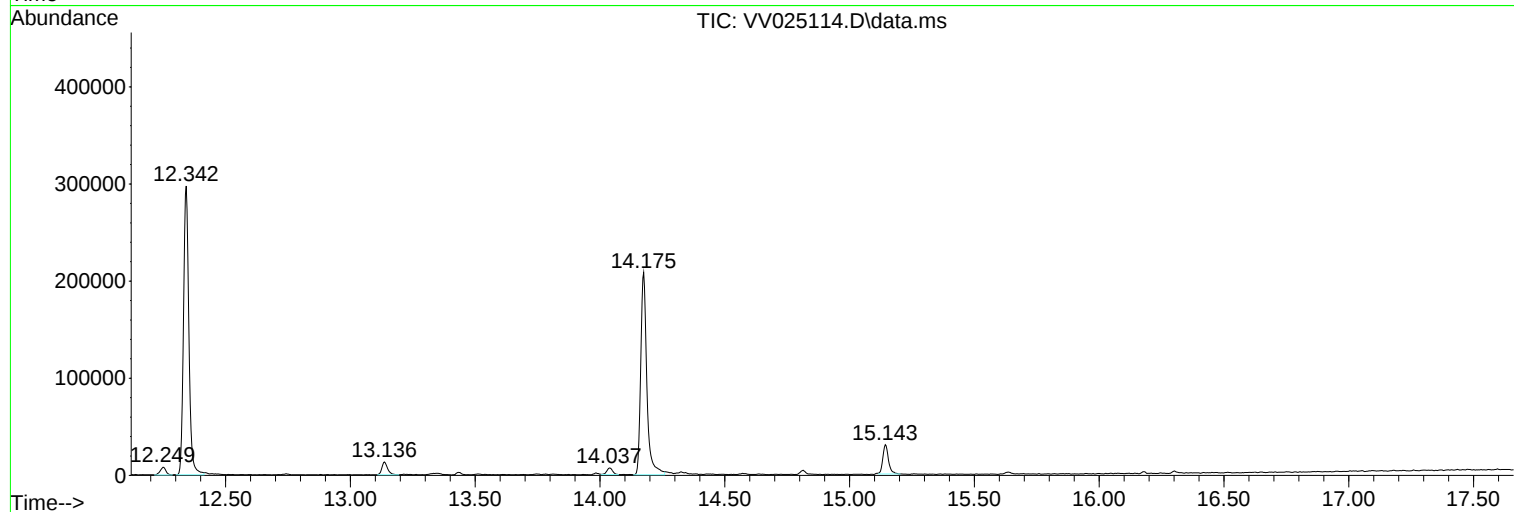
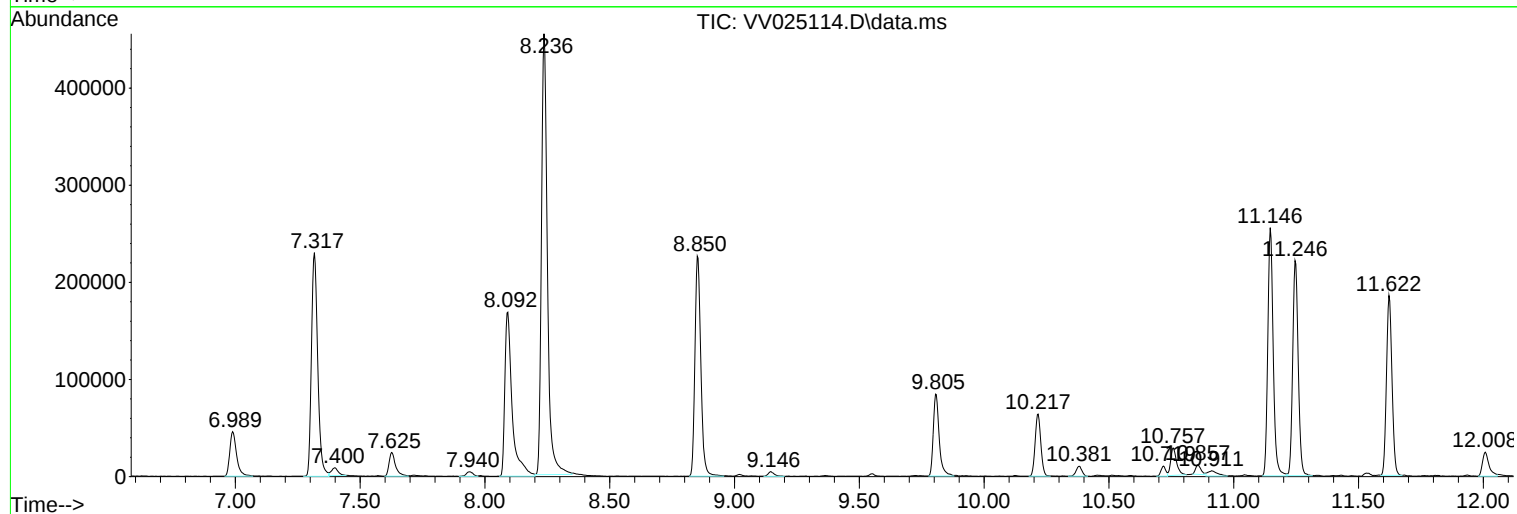
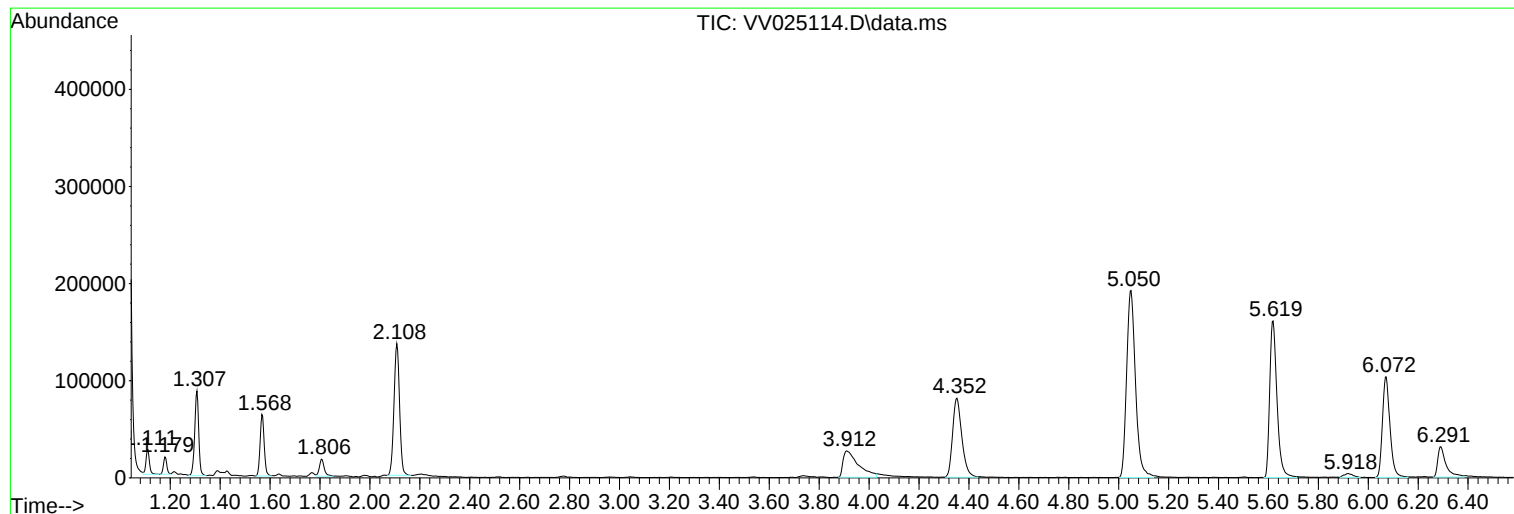
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR031522WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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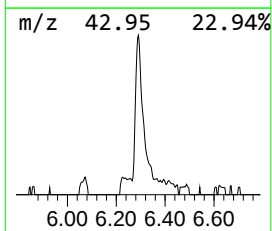
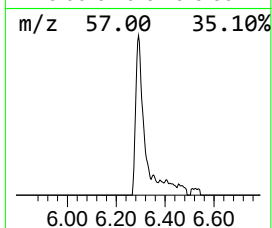
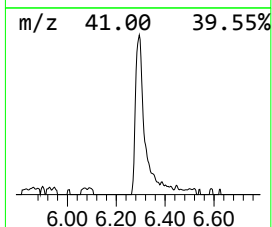
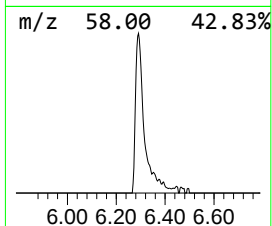
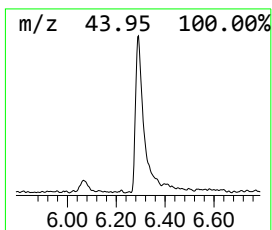
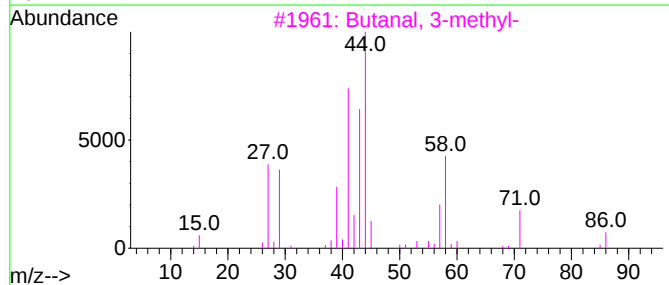
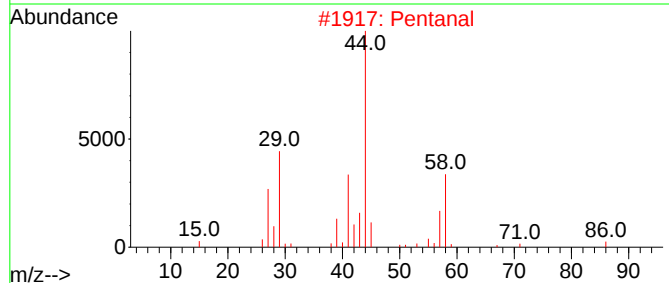
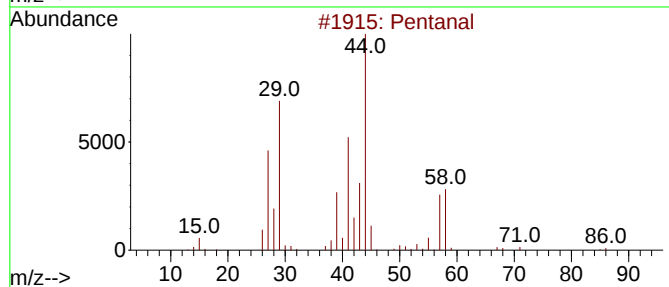
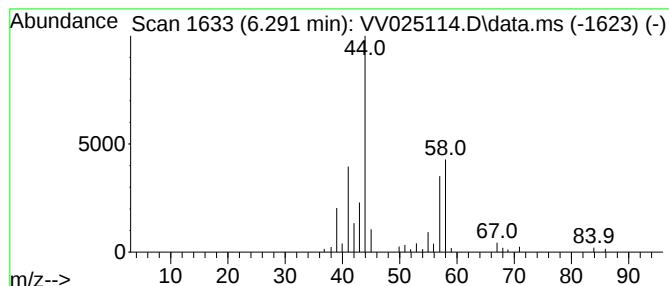
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.291	1.09 ug/L	71764	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	86
2	Pentanal			86	C5H10O	000110-62-3	83
3	Butanal, 3-methyl-			86	C5H10O	000590-86-3	64
4	Pentanal			86	C5H10O	000110-62-3	64
5	1-Octadecanamine, N-methyl-			283	C19H41N	002439-55-6	43



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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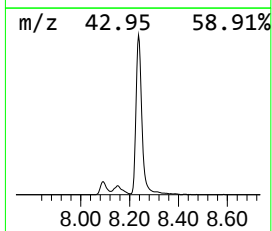
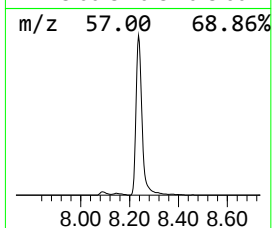
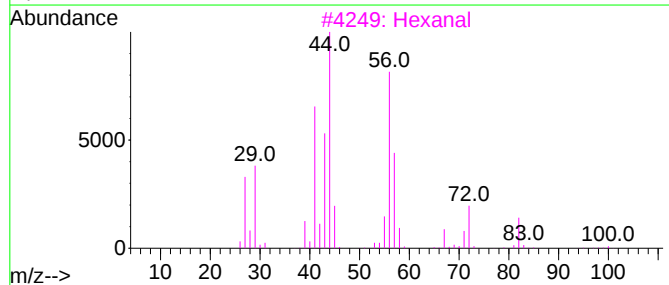
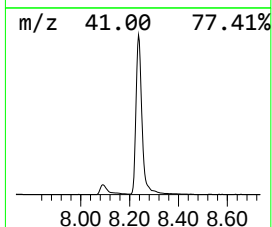
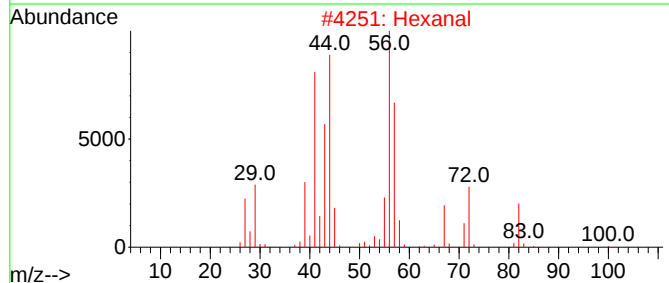
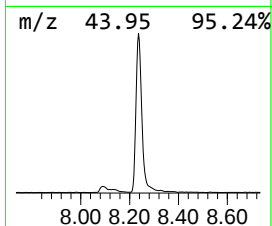
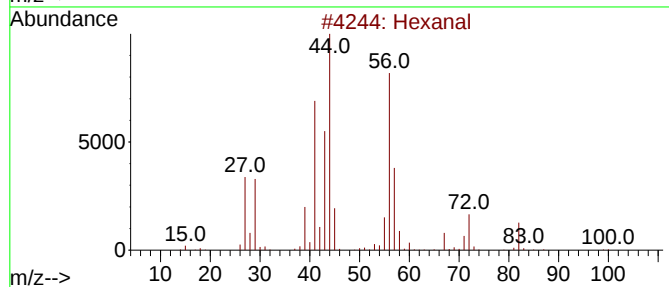
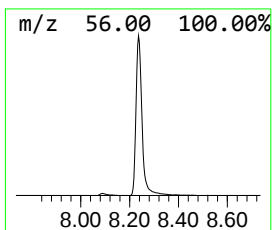
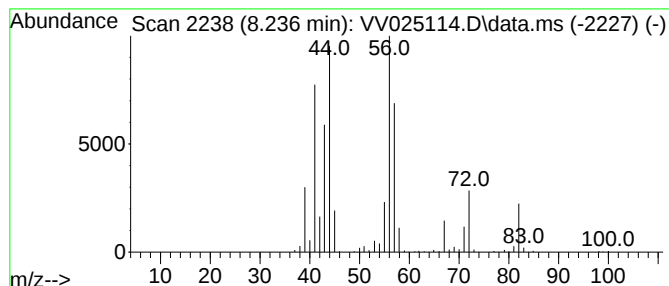
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR031522WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.236	10.14 ug/L	758858	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	94
2	Hexanal			100	C6H12O	000066-25-1	93
3	Hexanal			100	C6H12O	000066-25-1	91
4	Hexanal			100	C6H12O	000066-25-1	90
5	Hexanal			100	C6H12O	000066-25-1	83



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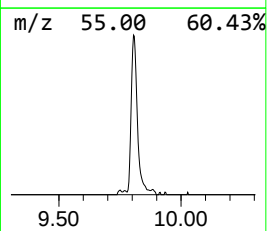
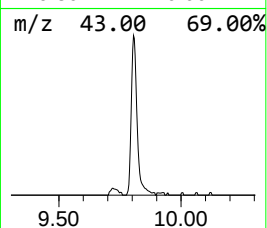
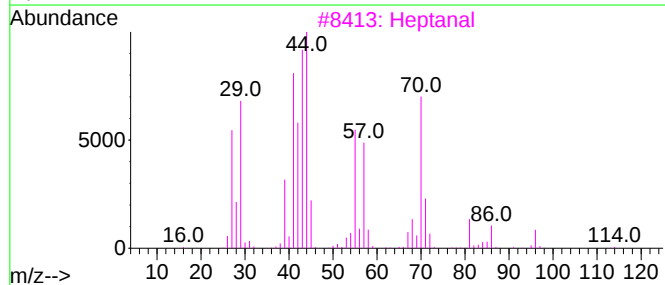
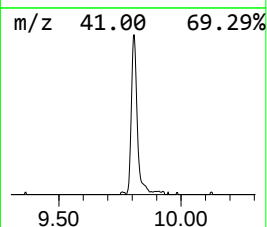
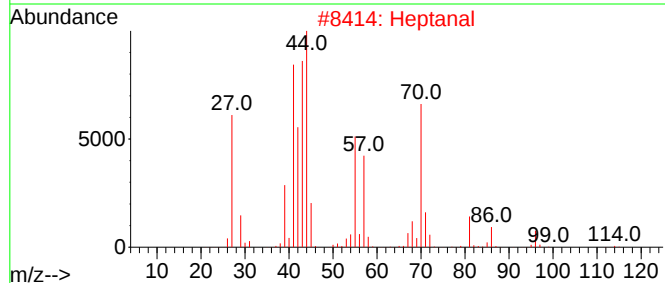
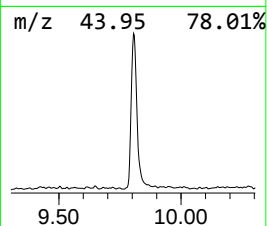
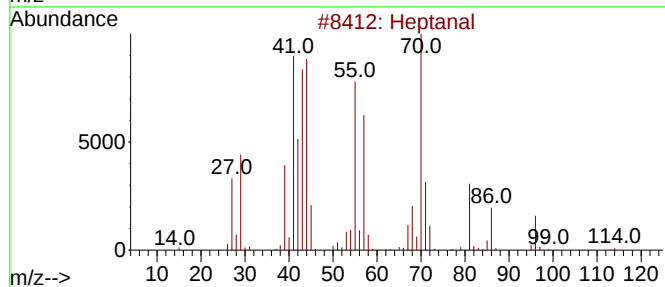
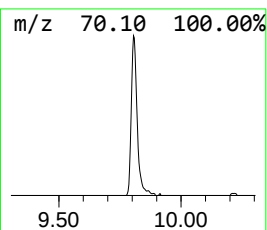
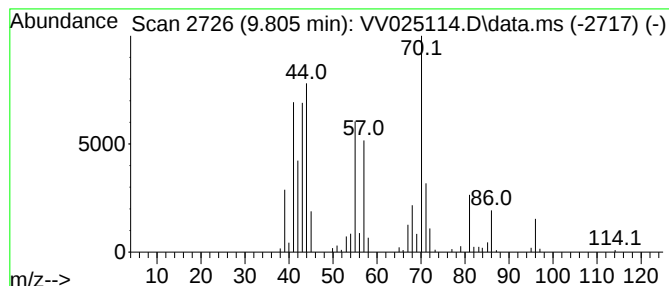
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Heptanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.805	1.85 ug/L	138783	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	97
2	Heptanal			114	C7H14O	000111-71-7	95
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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ALS Vial : 10 Sample Multiplier: 1

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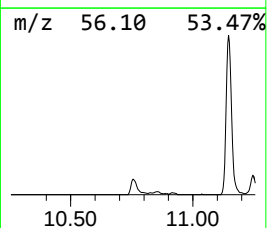
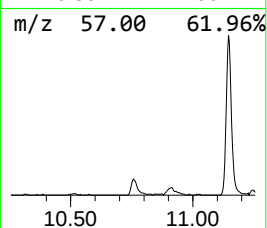
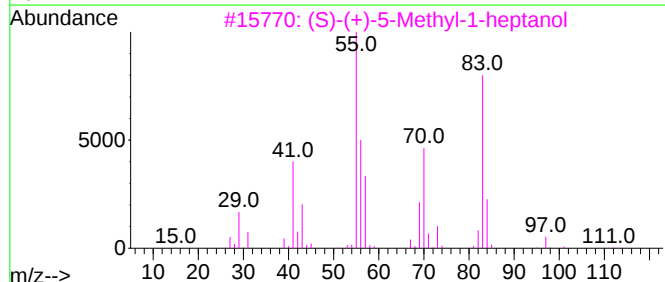
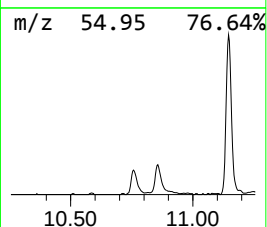
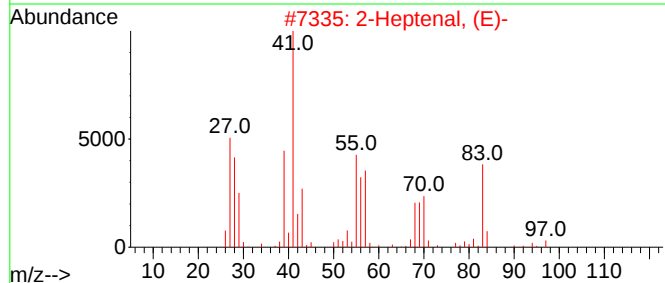
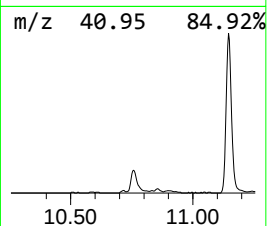
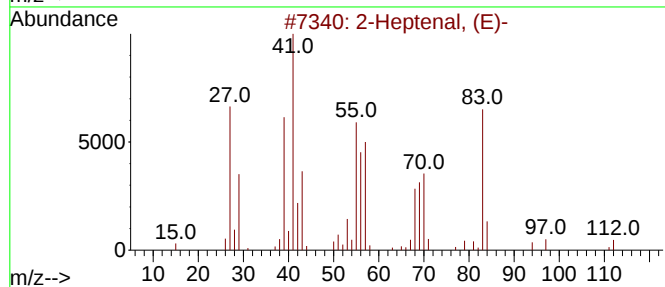
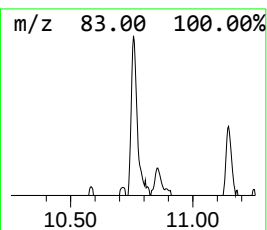
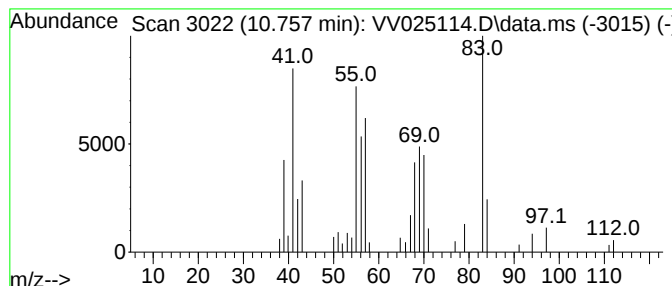
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Heptenal, (E)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.757	0.68 ug/L	46159	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptenal, (E)-	112	C7H12O	018829-55-5	94
2			2-Heptenal, (E)-	112	C7H12O	018829-55-5	83
3			(S)-(+)-5-Methyl-1-heptanol	130	C8H18O	057803-73-3	47
4			3-Ethylcyclopentanone	112	C7H12O	010264-55-8	46
5			Cyclopropane, octyl-	154	C11H22	001472-09-9	38



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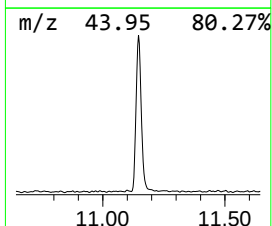
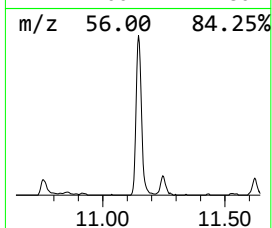
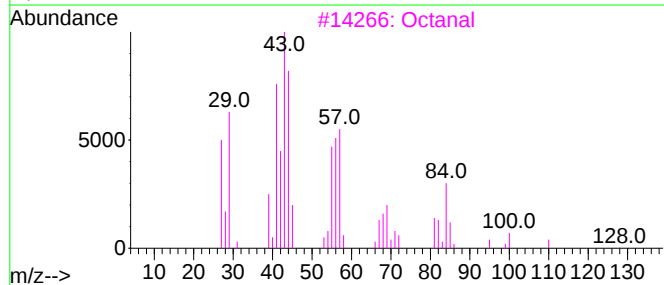
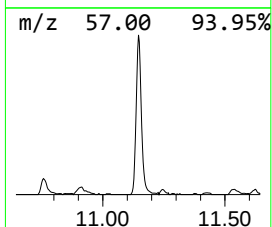
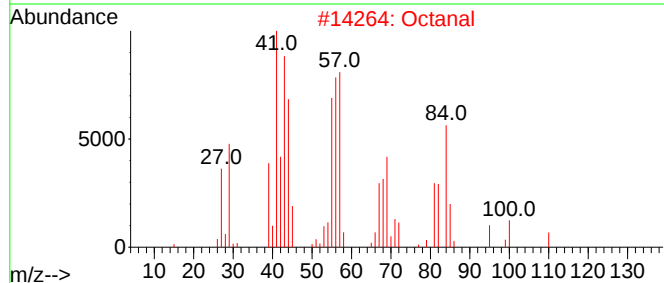
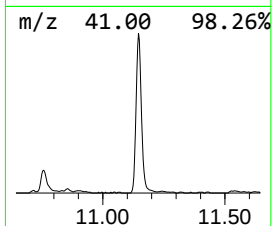
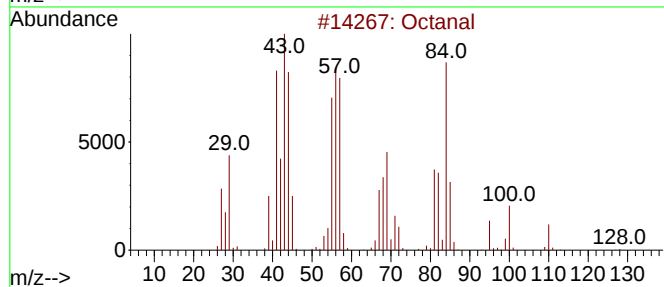
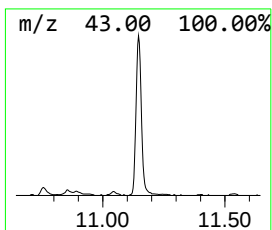
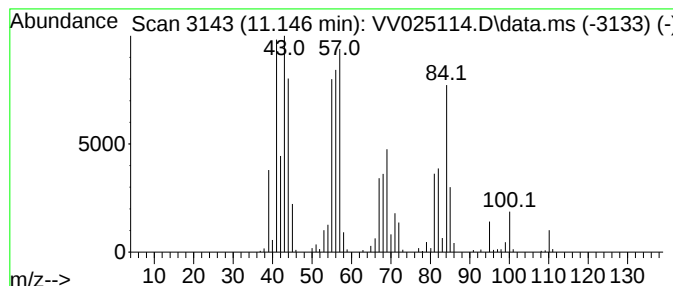
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.146	5.65 ug/L	385208	1,4-Dichlorobenzene-d4	11.246

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	78
5	Octanal			128	C8H16O	000124-13-0	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032122\
Data File : VV025114.D
Acq On : 21 Mar 2022 13:14
Operator : SY/MD
Sample : N2044-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFY28

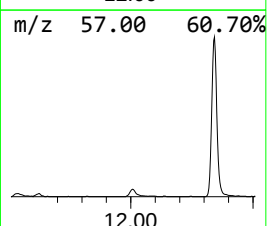
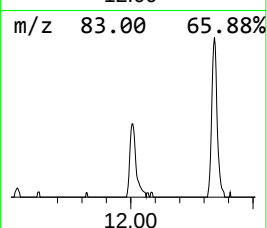
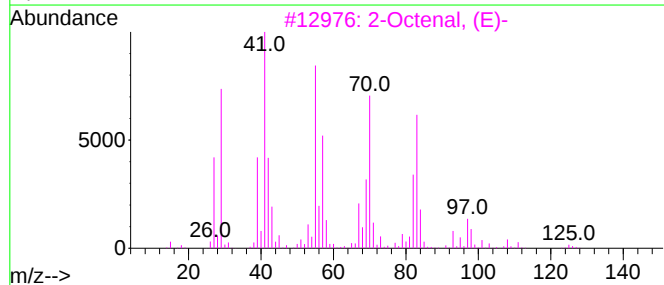
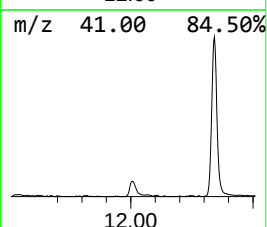
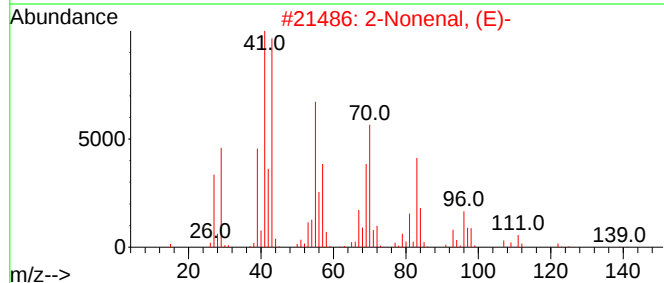
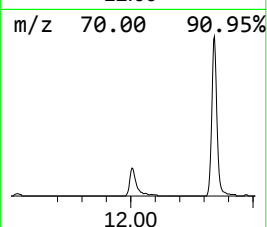
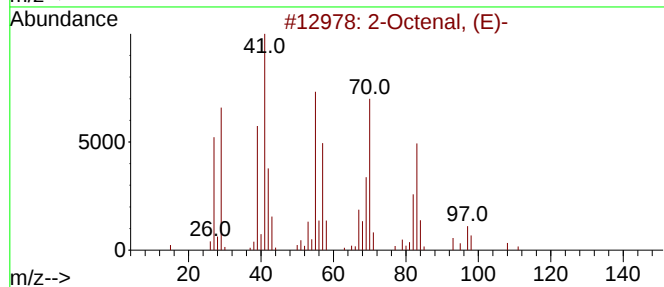
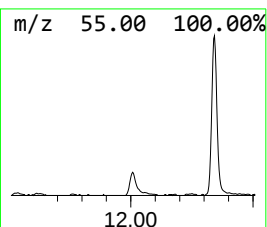
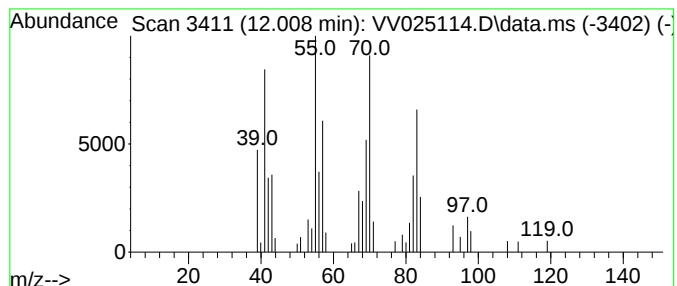
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 2-Octenal, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.008	0.67 ug/L	45356	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Octenal, (E)-	126	C8H14O	002548-87-0	72
2			2-Nonenal, (E)-	140	C9H16O	018829-56-6	50
3			2-Octenal, (E)-	126	C8H14O	002548-87-0	47
4			cis-2,4-Dimethylthiane, S,S-dioxide	162	C7H14O2S	1000215-67-5	43
5			Butane, 2-cyclopropyl-	98	C7H14	005750-02-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032122\
Data File : VV025114.D
Acq On : 21 Mar 2022 13:14
Operator : SY/MD
Sample : N2044-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

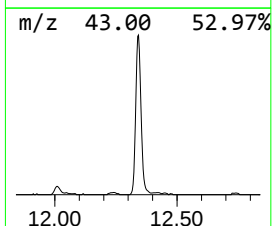
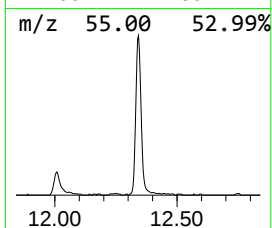
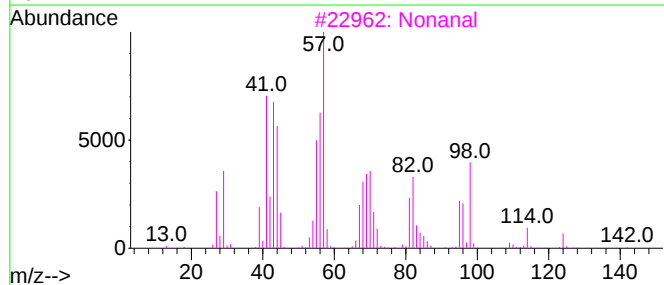
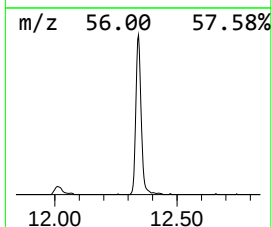
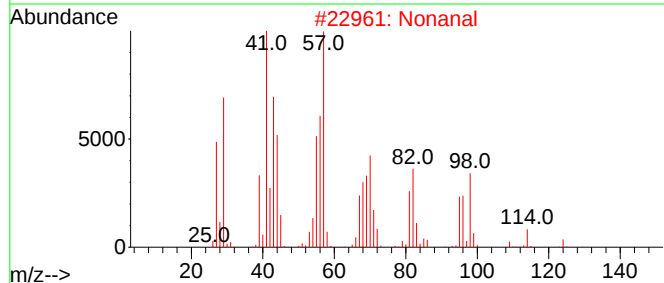
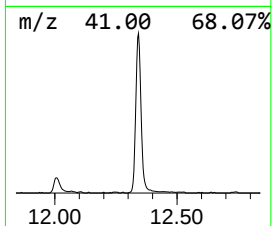
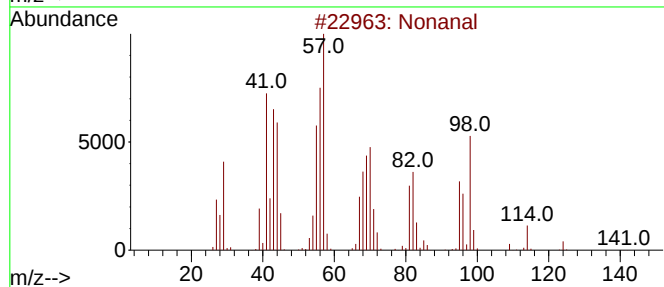
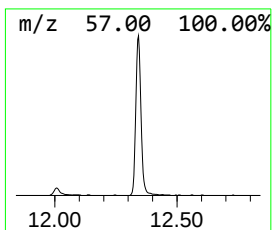
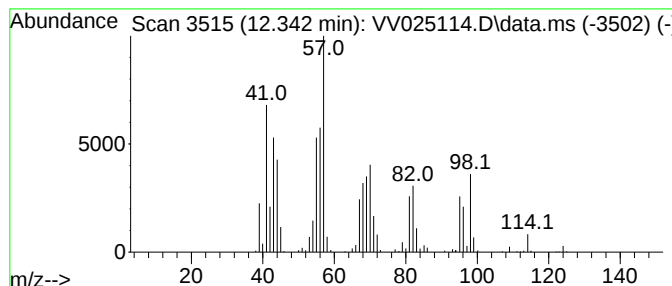
Instrument :
MSVOA_V
ClientSampleId :
BFY28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR031522WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
12.342	6.53 ug/L	444751	1,4-Dichlorobenzene-d4		11.246	
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	86
4	Nonanal		142	C9H18O	000124-19-6	83
5	2-Nonen-1-ol, (E)-		142	C9H18O	031502-14-4	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032122\
Data File : VV025114.D
Acq On : 21 Mar 2022 13:14
Operator : SY/MD
Sample : N2044-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFY28

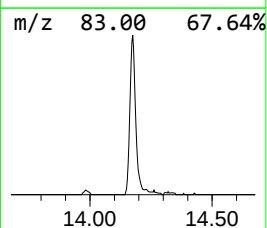
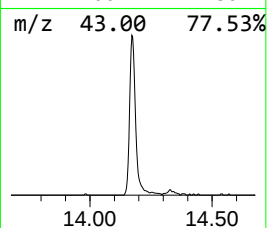
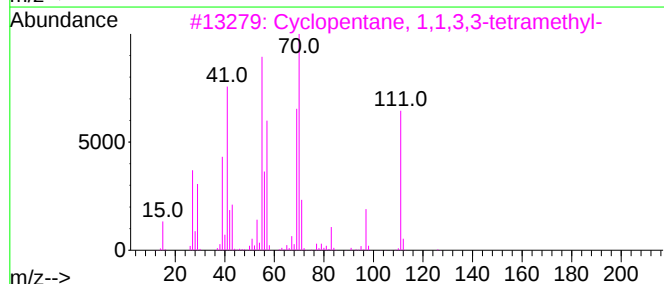
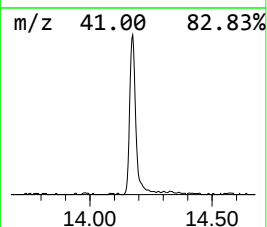
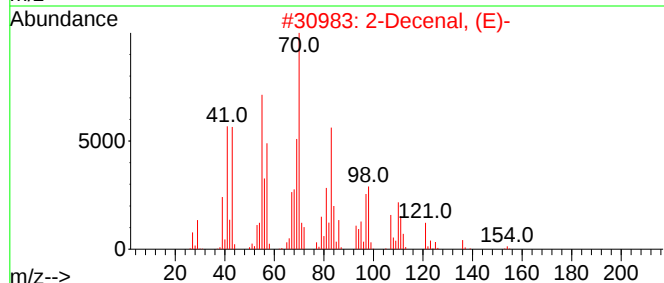
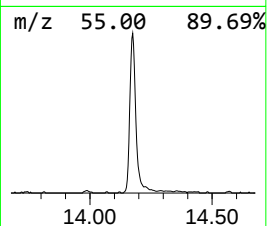
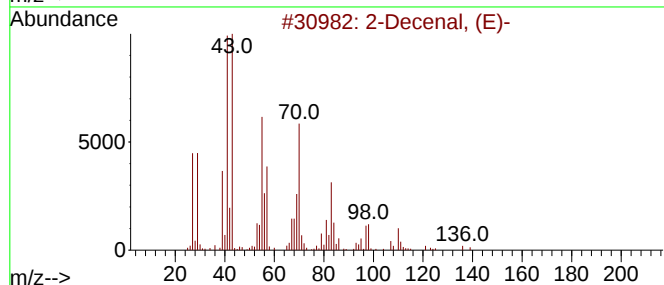
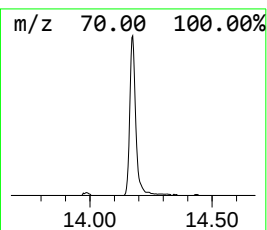
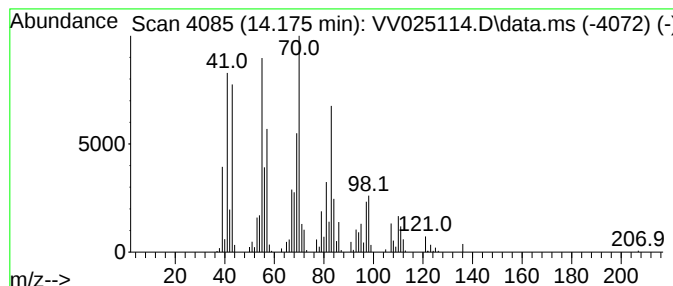
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 2-Decenal, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.175	5.21 ug/L	355209	1,4-Dichlorobenzene-d4	11.246

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	80
3			Cyclopentane, 1,1,3,3-tetramethyl-	126	C9H18	050876-33-0	55
4			2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	49
5			n-Heptadecanol-1	256	C17H36O	001454-85-9	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032122\
Data File : VV025114.D
Acq On : 21 Mar 2022 13:14
Operator : SY/MD
Sample : N2044-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFY28

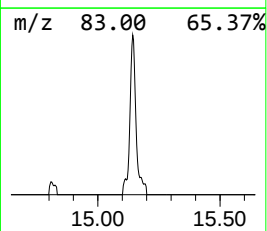
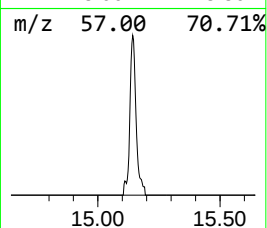
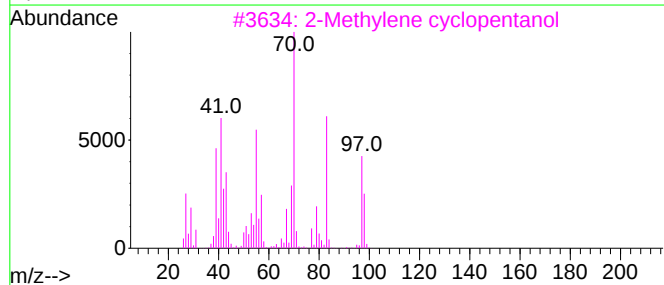
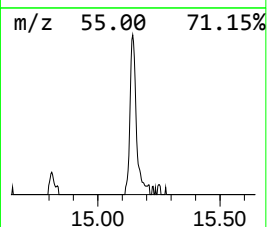
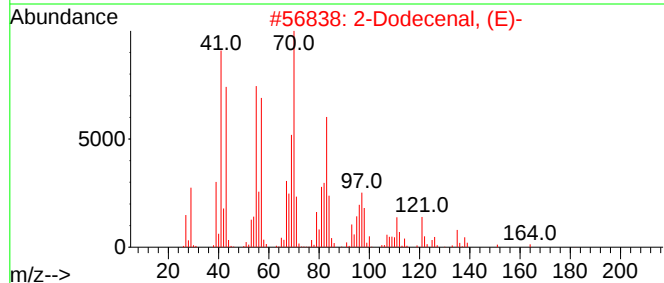
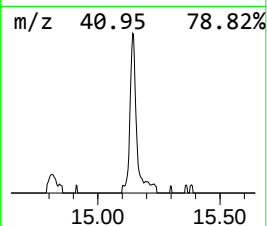
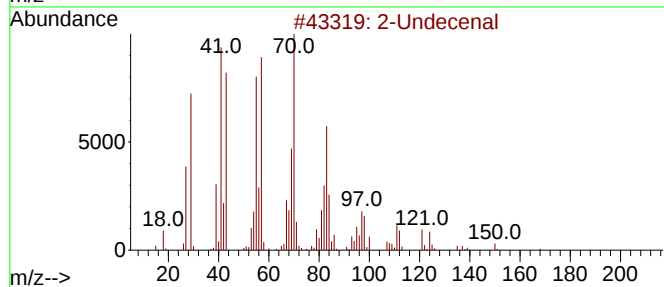
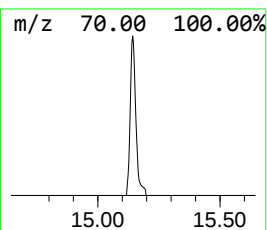
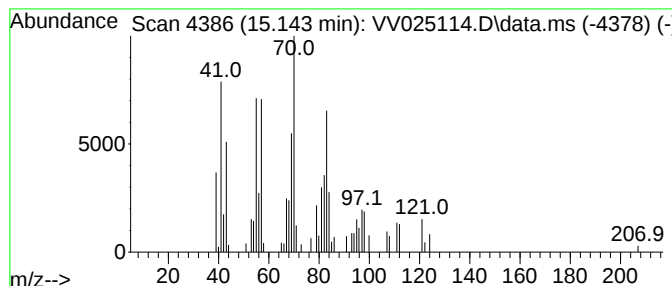
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR031522WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 2-Undecenal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.143	0.69 ug/L	47001	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Undecenal	168	C11H20O	002463-77-6	86
2			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	64
3			2-Methylene cyclopentanol	98	C6H10O	020461-31-8	49
4			2-Dodecenal, (E)-	182	C12H22O	020407-84-5	47
5			n-Pentadecanol	228	C15H32O	000629-76-5	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV032122\
 Data File : VV025114.D
 Acq On : 21 Mar 2022 13:14
 Operator : SY/MD
 Sample : N2044-04
 Misc : 25mL/MSVOA_V/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFY28

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR031522WMA.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	6.291	1.1	ug/L	71764	1	5.619	328064	5.0
Hexanal	8.236	10.1	ug/L	758858	2	8.850	374081	5.0
Heptanal	9.805	1.9	ug/L	138783	2	8.850	374081	5.0
2-Heptenal, (E)-	10.757	0.7	ug/L	46159	3	11.246	340660	5.0
Octanal	11.146	5.7	ug/L	385208	3	11.246	340660	5.0
2-Octenal, (E)-	12.008	0.7	ug/L	45356	3	11.246	340660	5.0
Nonanal	12.342	6.5	ug/L	444751	3	11.246	340660	5.0
2-Decenal, (E)-	14.175	5.2	ug/L	355209	3	11.246	340660	5.0
2-Undecenal	15.143	0.7	ug/L	47001	3	11.246	340660	5.0