

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
 Data File : VV032464.D
 Acq On : 18 Oct 2023 12:18
 Operator : SY/MD
 Sample : 04903-04
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AE7

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\SFAMVTR092923WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV032464.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.101	12	19	37	rVB2	189218	258842	54.09%	4.822%
2	1.178	37	43	49	rBV	6930	7583	1.58%	0.141%
3	1.220	50	56	60	rBV	17854	16710	3.49%	0.311%
4	1.320	71	87	102	rBV2	115335	189417	39.58%	3.529%
5	1.455	117	129	157	rBV4	24263	79869	16.69%	1.488%
6	1.645	180	188	203	rVB	50624	81302	16.99%	1.515%
7	1.728	206	214	221	rBV5	24024	42191	8.82%	0.786%
8	1.844	246	250	254	rBV6	10312	10906	2.28%	0.203%
9	2.265	372	381	396	rBV	113429	190139	39.73%	3.542%
10	4.484	1060	1071	1090	rVB	85165	197113	41.19%	3.672%
11	5.124	1257	1270	1289	rBV2	198777	439487	91.84%	8.187%
12	5.667	1429	1439	1452	rBV	120600	231577	48.39%	4.314%
13	5.982	1527	1537	1538	rBV9	6672	8830	1.85%	0.164%
14	6.217	1594	1610	1631	rVB	80925	179865	37.58%	3.351%
15	6.419	1664	1673	1694	rVB7	18164	43557	9.10%	0.811%
16	7.059	1861	1872	1892	rBV	40960	77714	16.24%	1.448%
17	7.310	1939	1950	1957	rBV10	4201	9824	2.05%	0.183%
18	7.371	1958	1969	1980	rBV	171845	300357	62.76%	5.595%
19	7.493	2002	2007	2018	rVB2	10725	17803	3.72%	0.332%
20	7.661	2050	2059	2072	rBV2	22840	42827	8.95%	0.798%
21	7.960	2141	2152	2157	rBV	11193	18692	3.91%	0.348%
22	8.001	2157	2165	2176	rVB3	20645	33951	7.09%	0.632%
23	8.117	2185	2201	2237	rBV	154931	478559	100.00%	8.915%
24	8.259	2237	2245	2262	rVB2	64053	114109	23.84%	2.126%
25	8.847	2417	2428	2459	rBV	172195	352960	73.75%	6.575%
26	9.008	2470	2478	2481	rBV5	3944	4853	1.01%	0.090%
27	9.127	2505	2515	2533	rBV2	13752	33552	7.01%	0.625%
28	9.217	2534	2543	2561	rVB4	10855	27197	5.68%	0.507%
29	9.371	2585	2591	2601	rBV3	6391	9779	2.04%	0.182%
30	9.525	2631	2639	2647	rBV	7325	14068	2.94%	0.262%
31	9.696	2680	2692	2704	rBV6	8288	20088	4.20%	0.374%
32	9.783	2708	2719	2745	rVV2	54332	114418	23.91%	2.131%
33	10.185	2833	2844	2862	rVB	59513	114911	24.01%	2.141%
34	10.345	2882	2894	2903	rVB3	17710	33567	7.01%	0.625%
35	10.416	2908	2916	2919	rBV8	4993	6133	1.28%	0.114%
36	10.471	2925	2933	2950	rVB4	25120	51578	10.78%	0.961%

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37	10.554	2952	2959	2960	rBV4	4343	4830	1.01%	0.090%
38	10.705	2999	3006	3014	rVB4	2834	6484	1.35%	0.121%
39	10.879	3049	3060	3075	rVB	14327	28965	6.05%	0.540%
40	11.001	3091	3098	3112	rBV2	8945	16703	3.49%	0.311%
41	11.107	3122	3131	3151	rBV2	57699	104319	21.80%	1.943%
42	11.204	3151	3161	3181	rVB	205775	348172	72.75%	6.486%
43	11.496	3232	3252	3268	rBV4	54719	175920	36.76%	3.277%
44	11.577	3268	3277	3304	rVB	206643	403081	84.23%	7.509%
45	11.786	3337	3342	3355	rVB3	19366	33813	7.07%	0.630%
46	11.866	3360	3367	3370	rBV6	6367	8997	1.88%	0.168%
47	11.969	3392	3399	3416	rVB4	11320	24416	5.10%	0.455%
48	12.201	3459	3471	3483	rBV3	19728	40555	8.47%	0.755%
49	12.294	3490	3500	3515	rBV	58725	96037	20.07%	1.789%
50	12.365	3516	3522	3529	rVV2	8286	12648	2.64%	0.236%
51	12.413	3529	3537	3550	rVB	13006	23044	4.82%	0.429%
52	12.676	3613	3619	3625	rBV7	7187	11026	2.30%	0.205%
53	12.799	3649	3657	3659	rBV8	5218	6259	1.31%	0.117%
54	12.828	3662	3666	3682	rVB5	12079	21009	4.39%	0.391%
55	13.085	3738	3746	3763	rBV8	14912	28495	5.95%	0.531%
56	13.165	3765	3771	3779	rVB9	3742	5326	1.11%	0.099%
57	13.217	3779	3787	3793	rBV10	5841	8776	1.83%	0.163%
58	13.381	3835	3838	3851	rVB10	8001	11931	2.49%	0.222%
59	13.448	3853	3859	3870	rVB2	9236	14572	3.04%	0.271%
60	13.988	4016	4027	4036	rBV2	11496	18572	3.88%	0.346%
61	14.387	4145	4151	4160	rVB9	3968	5917	1.24%	0.110%
62	14.580	4205	4211	4218	rVB9	4661	5995	1.25%	0.112%
63	14.763	4260	4268	4277	rBV9	3455	5421	1.13%	0.101%
64	15.059	4343	4360	4364	rBV9	9434	26272	5.49%	0.489%
65	17.043	4970	4977	4985	rVB	11413	16224	3.39%	0.302%

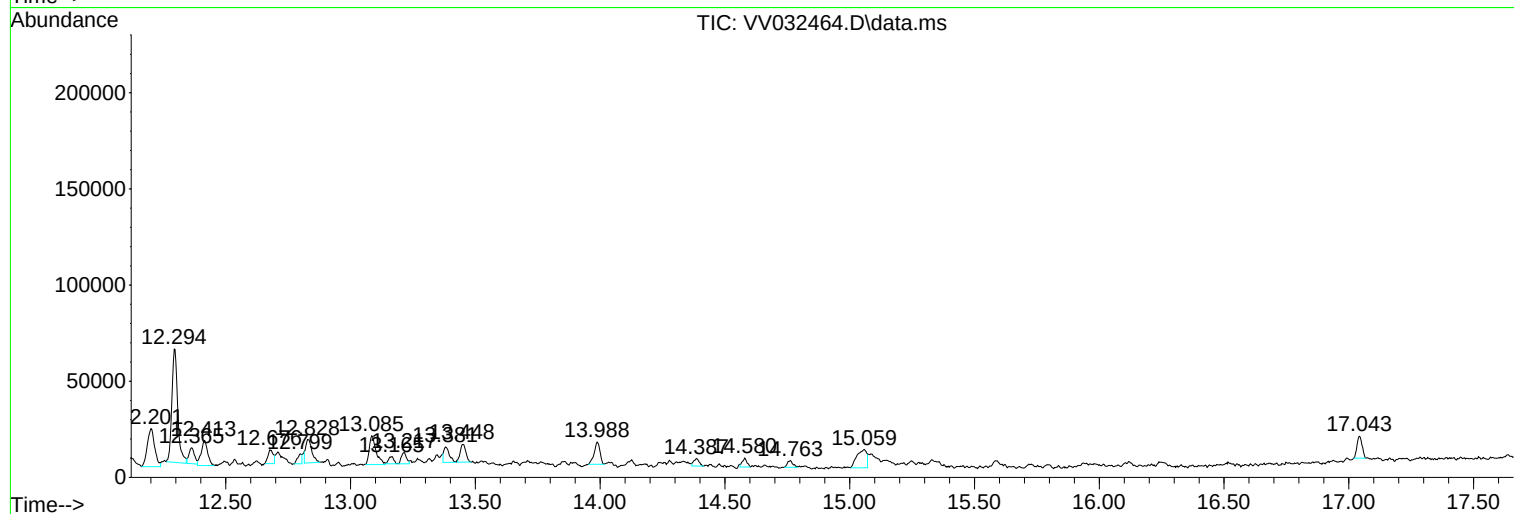
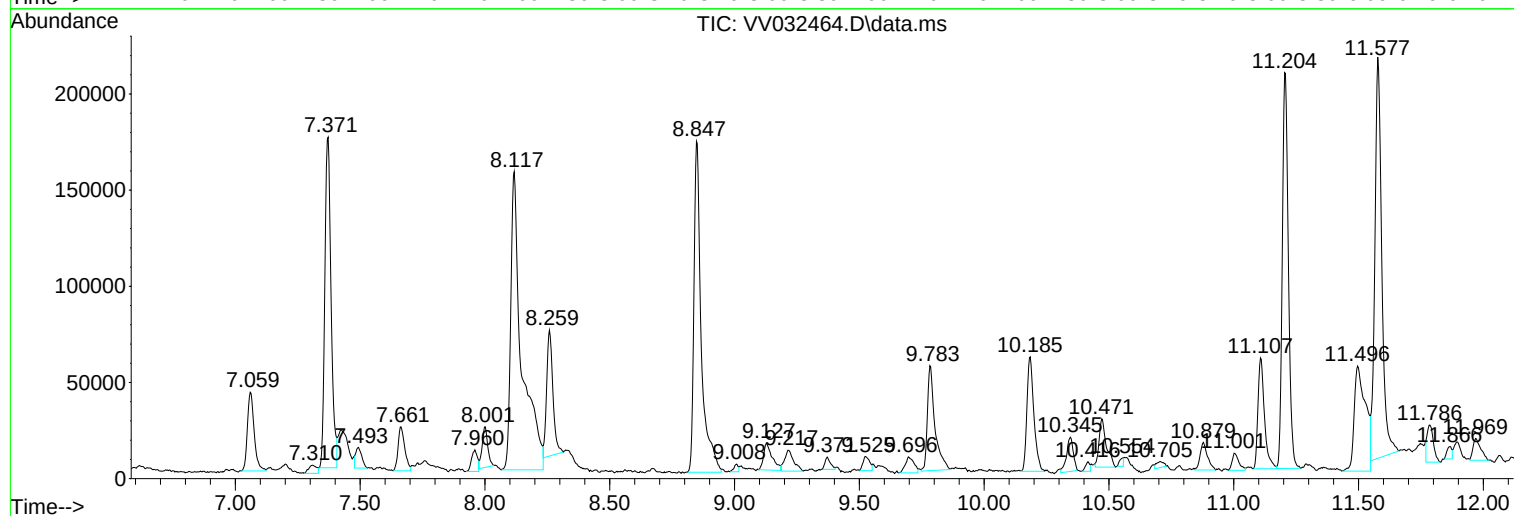
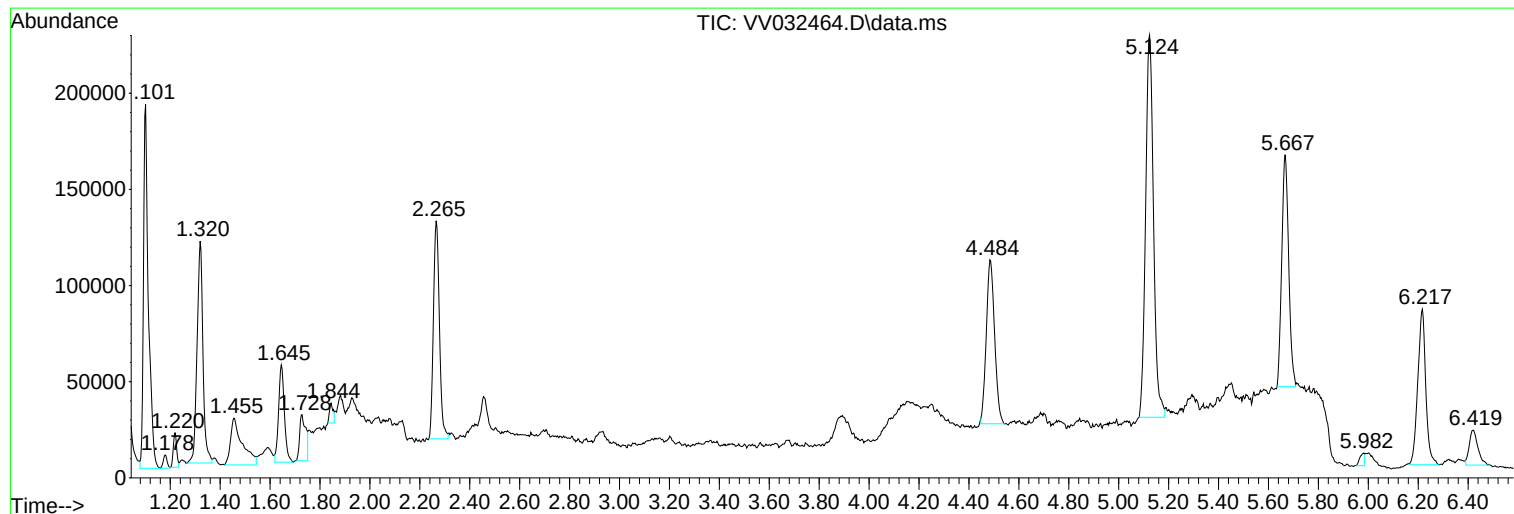
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Quant Title : TRACE VOA SFAM1.0

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



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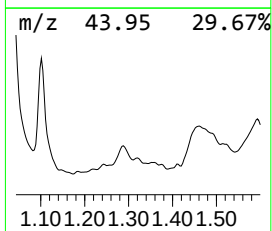
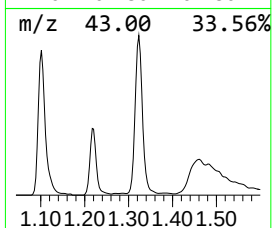
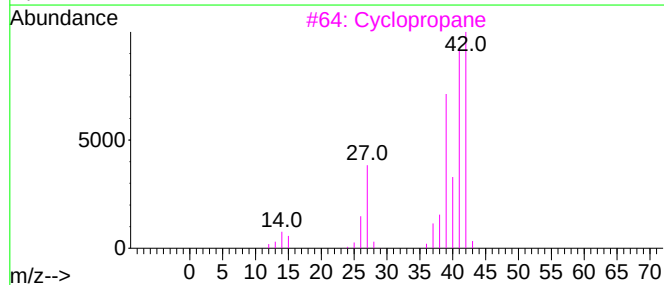
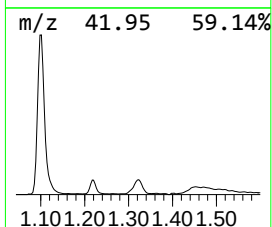
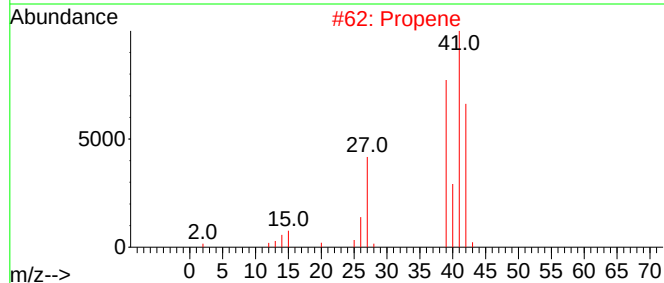
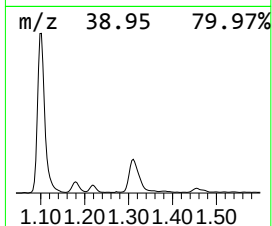
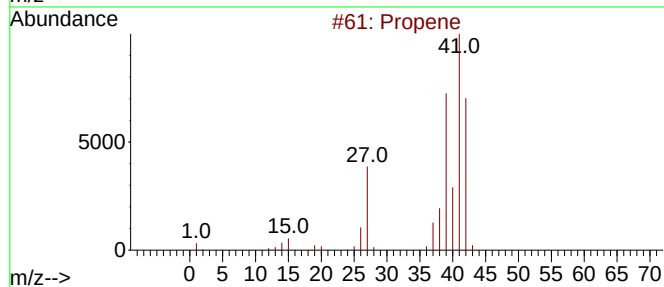
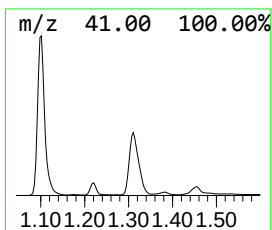
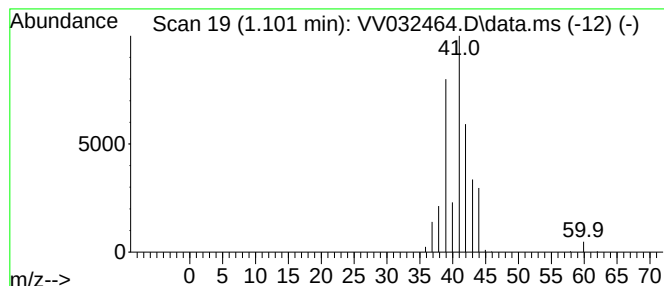
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.101	5.59 ug/L	258842	1,4-Difluorobenzene	5.667

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			Cyclopropane	42	C3H6	000075-19-4	7
5			Cyclopropene	40	C3H4	002781-85-3	5



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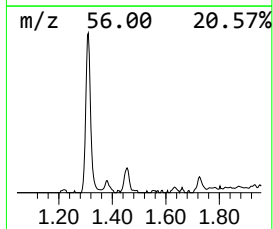
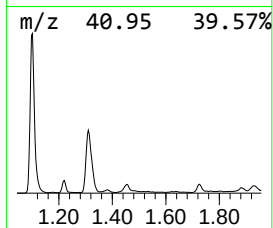
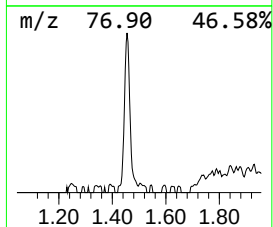
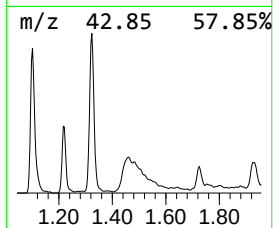
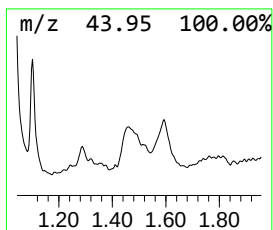
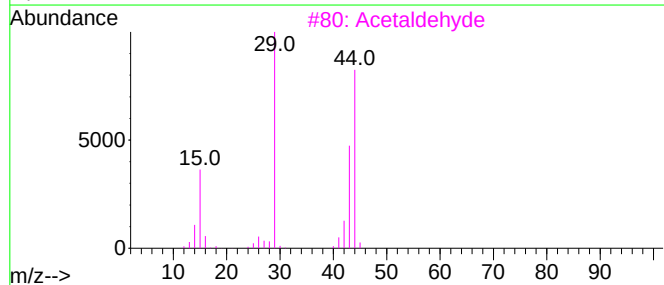
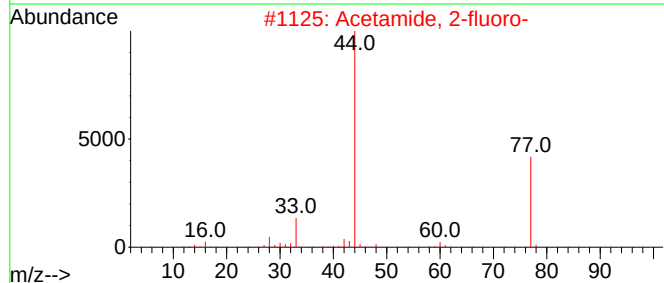
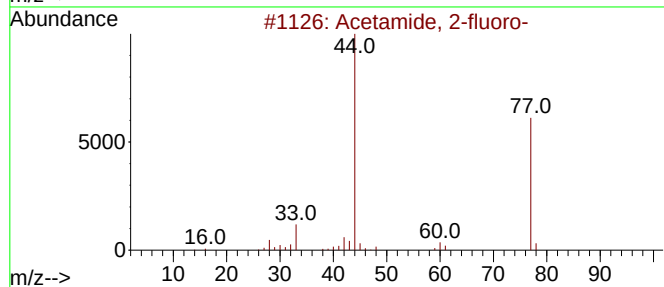
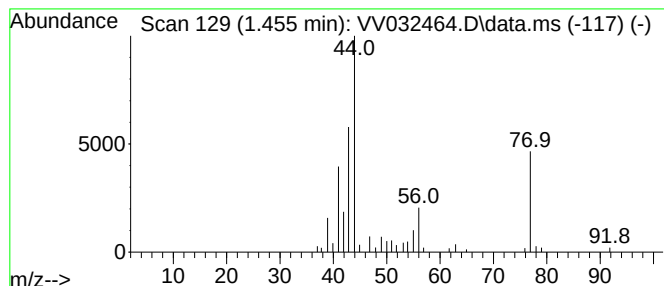
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Acetamide, 2-fluoro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.455	1.72 ug/L	79869	1,4-Difluorobenzene	5.667

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetamide, 2-fluoro-	77	C2H4FN0	000640-19-7	53
2			Acetamide, 2-fluoro-	77	C2H4FN0	000640-19-7	9
3			Acetaldehyde	44	C2H4O	000075-07-0	9
4			Acetaldehyde	44	C2H4O	000075-07-0	9
5			Propane	44	C3H8	000074-98-6	9



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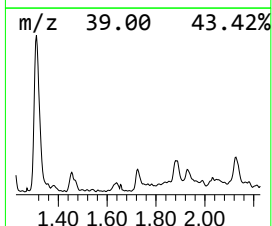
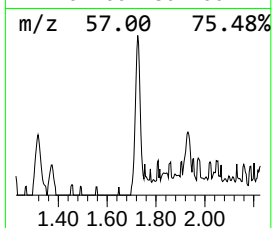
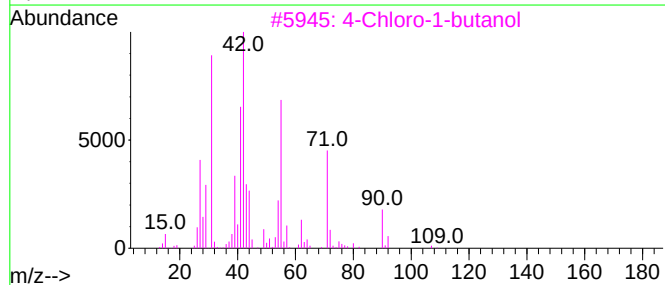
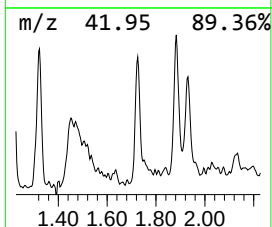
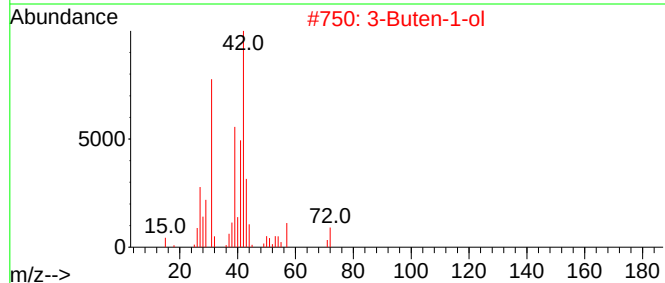
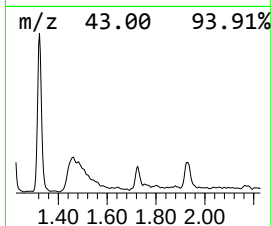
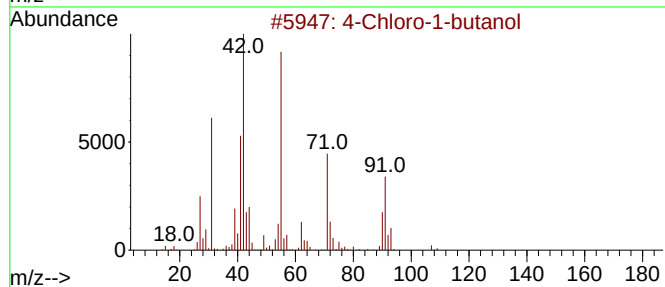
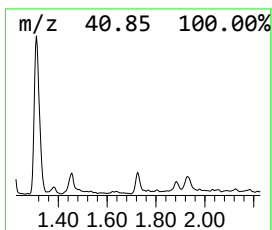
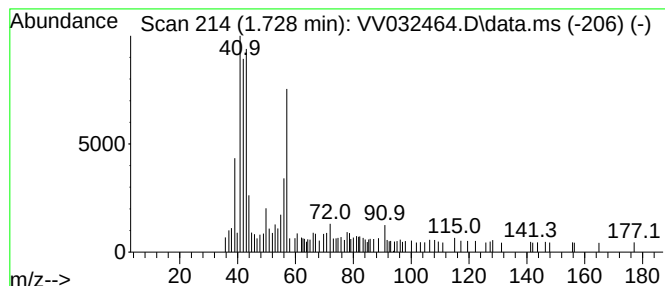
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 4-Chloro-1-butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.728	0.91 ug/L	42191	1,4-Difluorobenzene	5.667

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Chloro-1-butanol	108	C4H9ClO	000928-51-8	50
2			3-Buten-1-ol	72	C4H8O	000627-27-0	47
3			4-Chloro-1-butanol	108	C4H9ClO	000928-51-8	40
4			Thietane, 1-oxide	90	C3H6OS	013153-11-2	37
5			2-Chloro-2-propen-1-ol	92	C3H5ClO	005976-47-6	27



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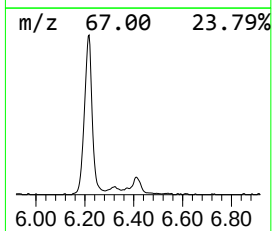
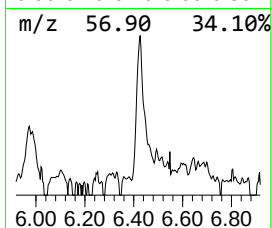
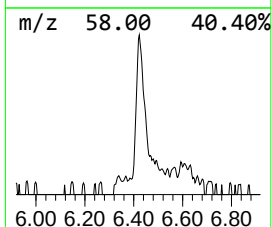
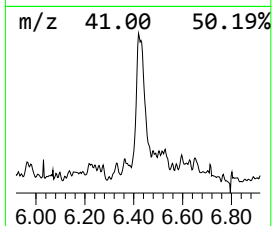
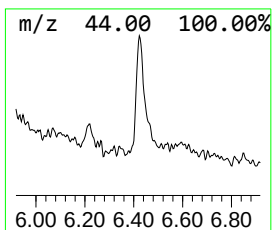
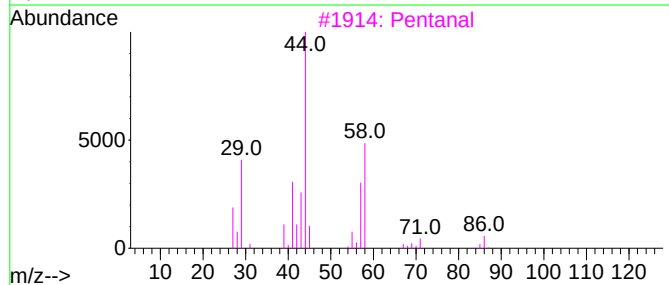
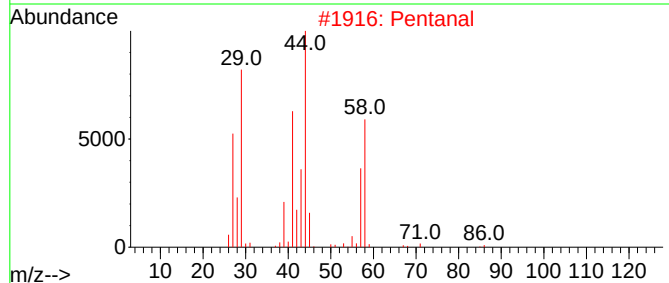
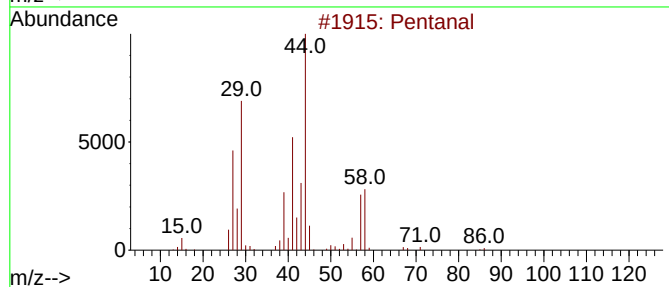
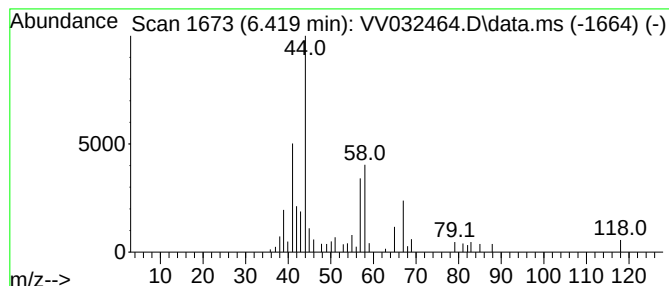
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.419	0.94 ug/L	43557	1,4-Difluorobenzene	5.667

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	53
2	Pentanal			86	C5H10O	000110-62-3	42
3	Pentanal			86	C5H10O	000110-62-3	36
4	1-Pentanol, 4-amino-			103	C5H13NO	000927-55-9	28
5	2-Formylhistamine			139	C6H9N3O	1000132-95-8	25



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Sample : 04903-04
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AE7

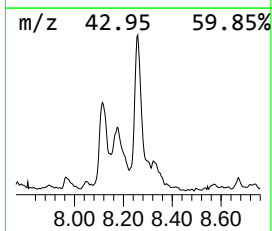
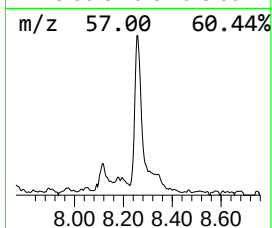
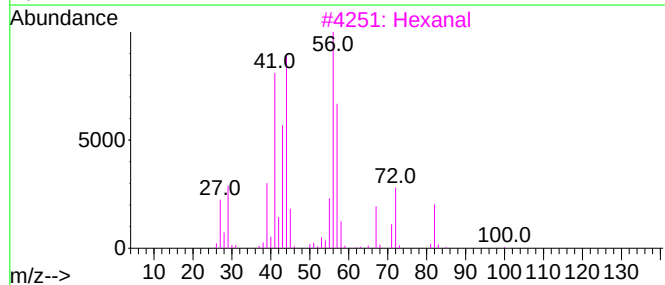
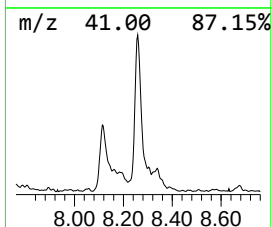
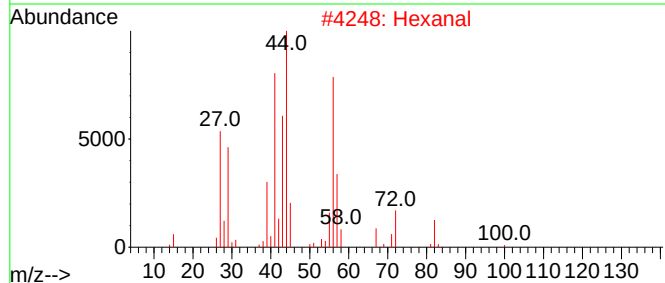
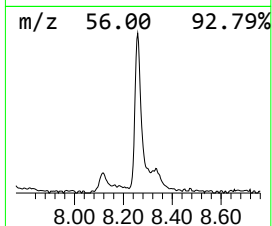
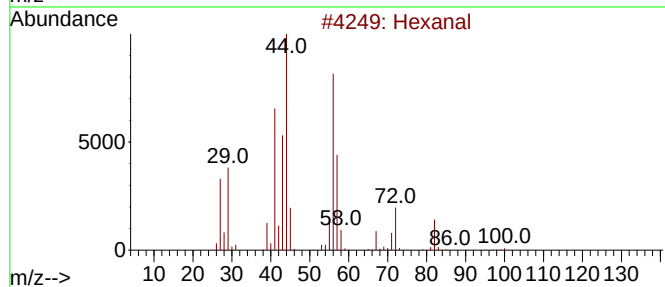
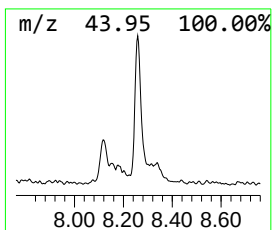
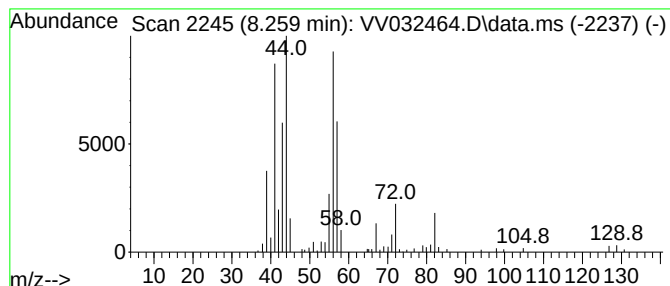
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.259	1.62 ug/L	114109	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	90
2	Hexanal			100	C6H12O	000066-25-1	90
3	Hexanal			100	C6H12O	000066-25-1	78
4	Hexanal			100	C6H12O	000066-25-1	72
5	Hexanal			100	C6H12O	000066-25-1	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
Data File : VV032464.D
Acq On : 18 Oct 2023 12:18
Operator : SY/MD
Sample : 04903-04
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AE7

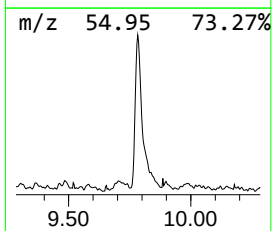
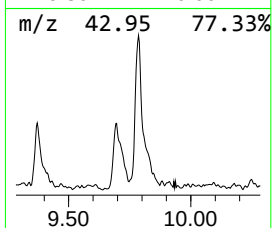
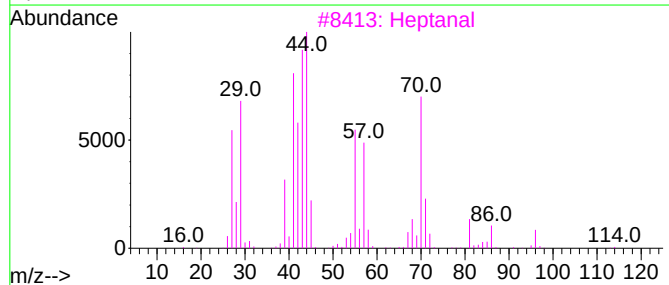
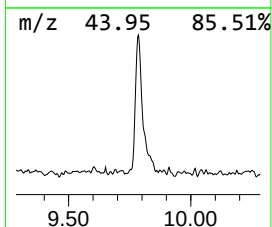
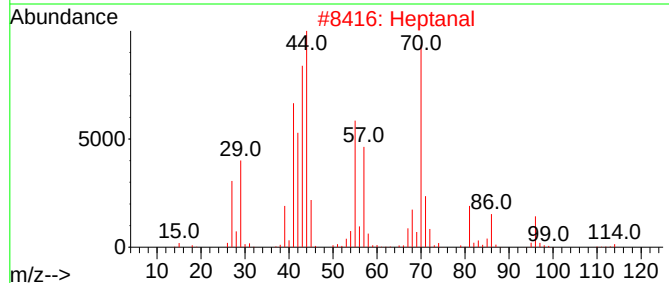
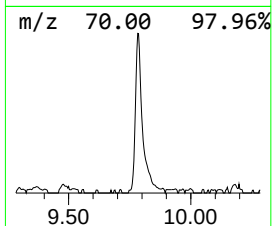
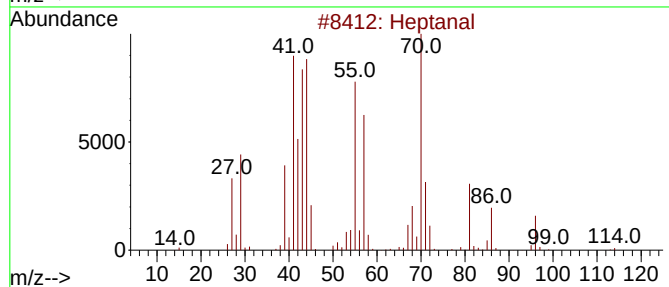
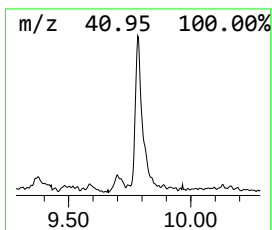
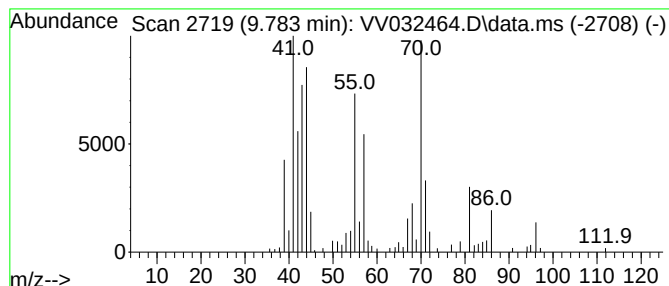
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Heptanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.783	1.62 ug/L	114418	Chlorobenzene-d5	8.847

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal			114	C7H14O	000111-71-7	91
2	Heptanal			114	C7H14O	000111-71-7	90
3	Heptanal			114	C7H14O	000111-71-7	83
4	Heptanal			114	C7H14O	000111-71-7	78
5	Heptanal			114	C7H14O	000111-71-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
Data File : VV032464.D
Acq On : 18 Oct 2023 12:18
Operator : SY/MD
Sample : 04903-04
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AE7

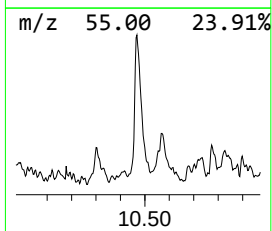
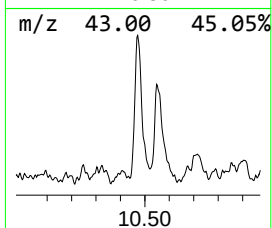
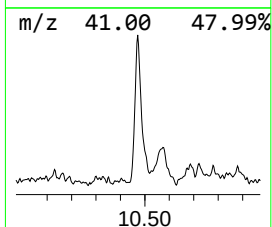
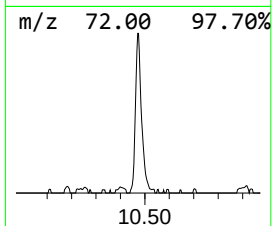
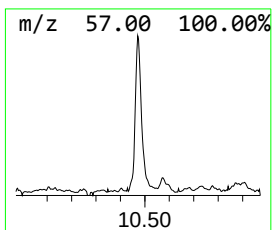
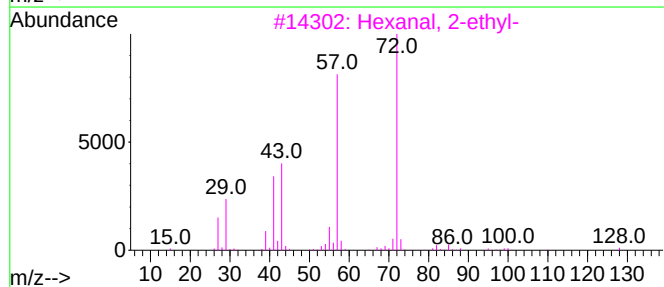
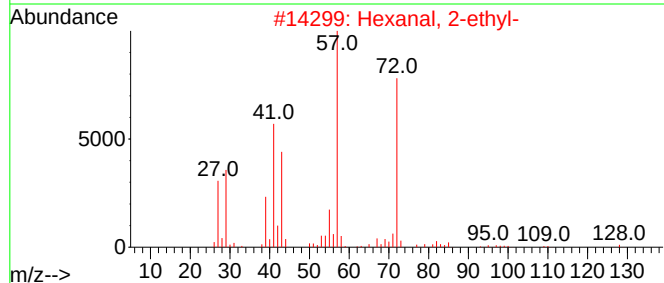
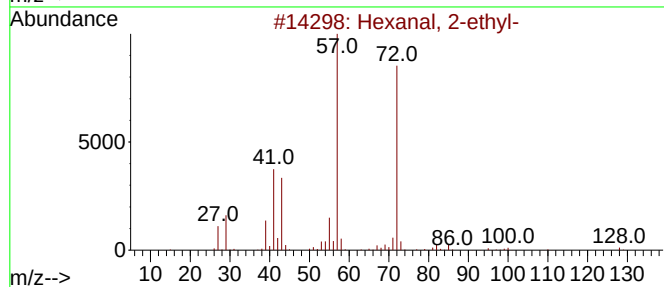
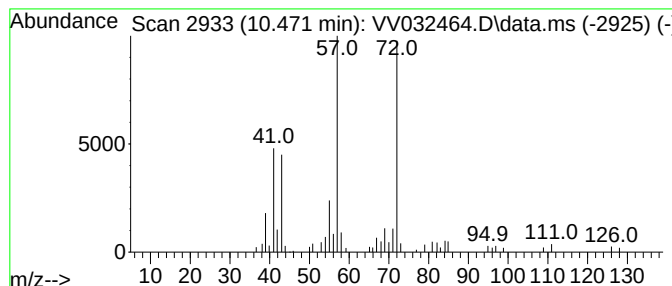
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Hexanal, 2-ethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.471	0.74 ug/L	51578	1,4-Dichlorobenzene-d4	11.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	87
2			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	83
3			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	64
4			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	56
5			(1R,2R)-(-)-N-Methylpseudoephedrine	179	C11H17NO	014222-20-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
Data File : VV032464.D
Acq On : 18 Oct 2023 12:18
Operator : SY/MD
Sample : 04903-04
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

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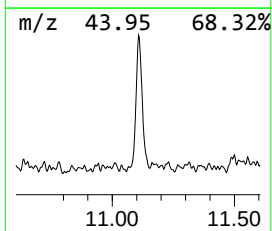
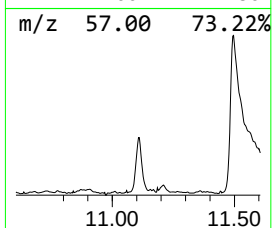
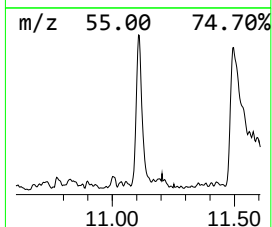
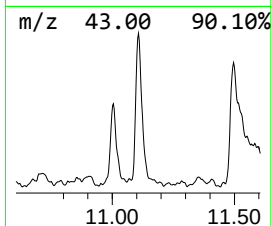
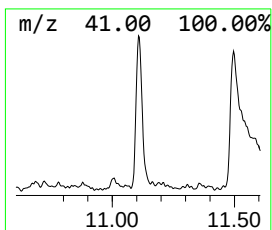
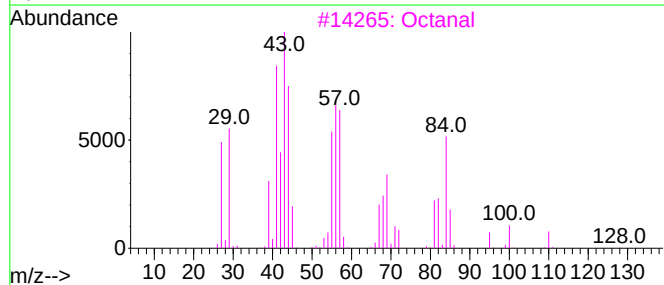
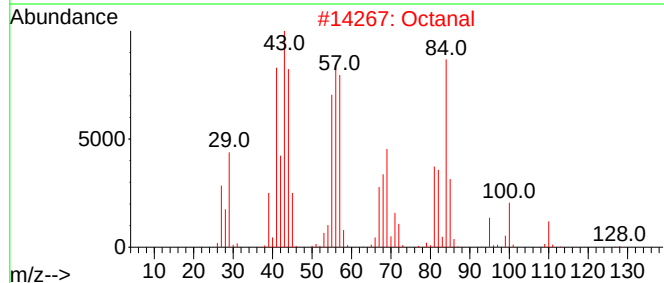
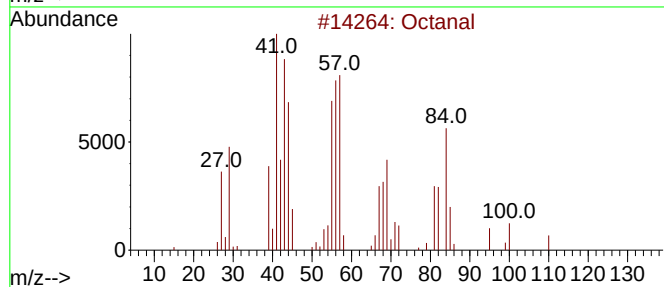
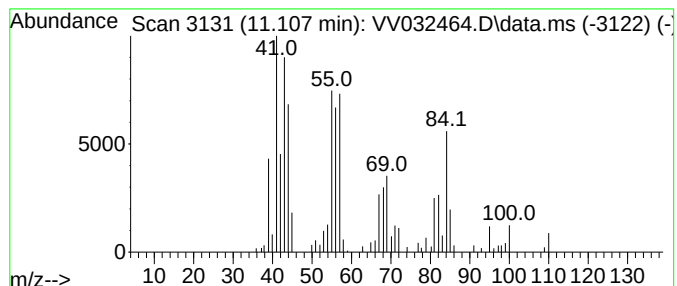
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Octanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.107	1.50 ug/L	104319	1,4-Dichlorobenzene-d4	11.207

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	91
4	Octanal			128	C8H16O	000124-13-0	90
5	Octanal			128	C8H16O	000124-13-0	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
Data File : VV032464.D
Acq On : 18 Oct 2023 12:18
Operator : SY/MD
Sample : 04903-04
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

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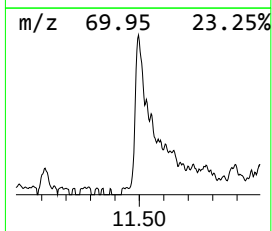
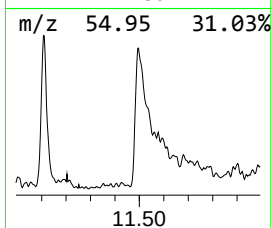
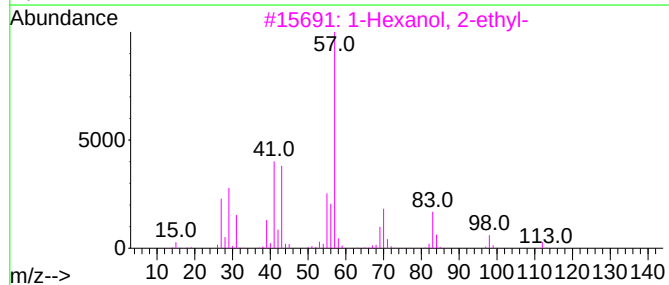
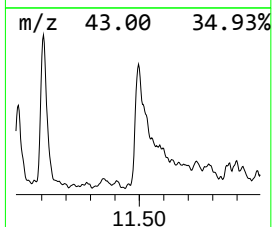
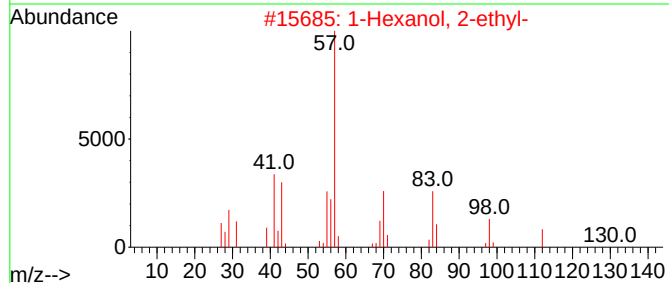
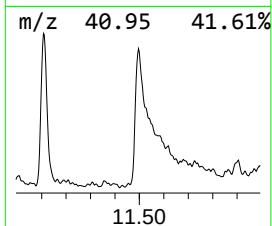
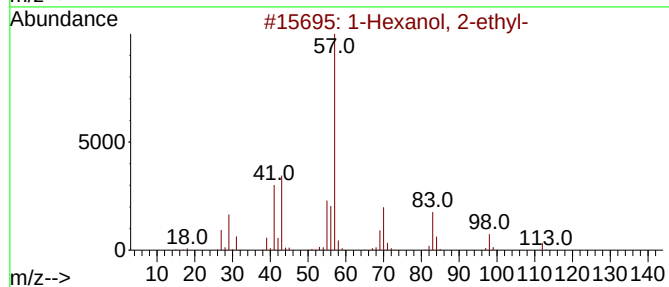
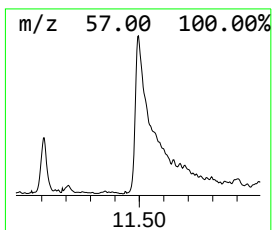
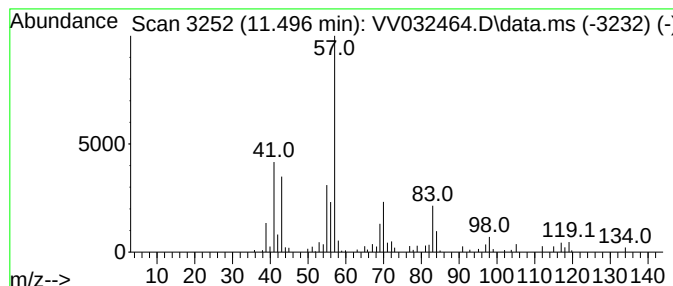
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.496	2.53 ug/L	175920	1,4-Dichlorobenzene-d4	11.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
Data File : VV032464.D
Acq On : 18 Oct 2023 12:18
Operator : SY/MD
Sample : 04903-04
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0AE7

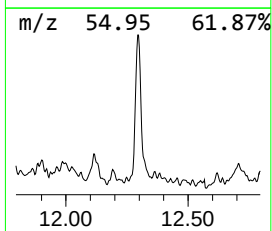
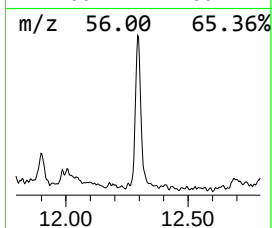
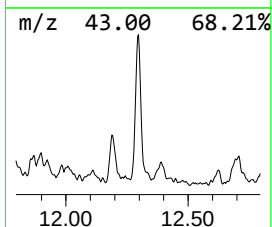
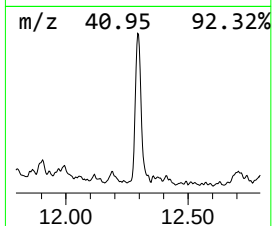
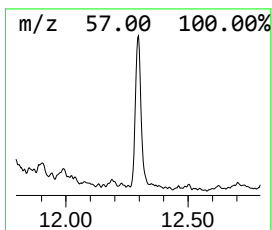
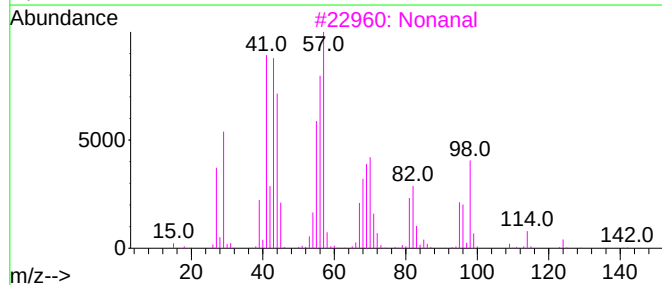
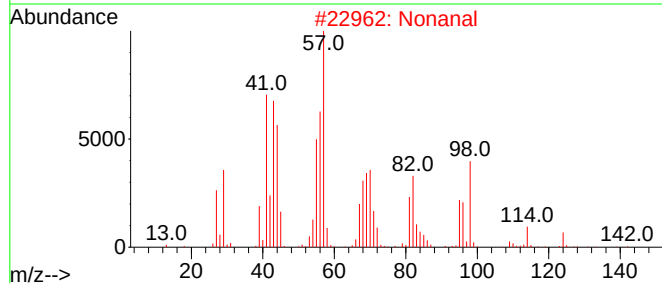
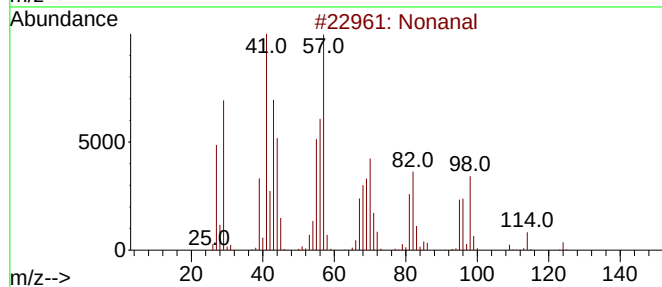
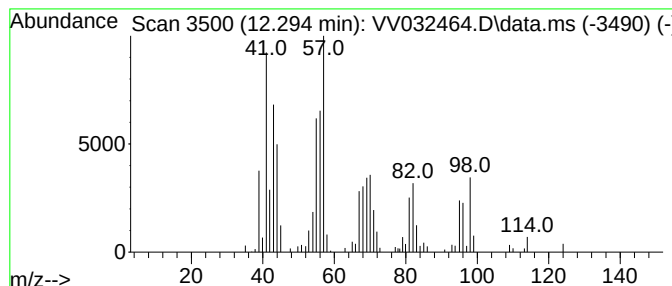
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 Nonanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.294	1.38 ug/L	96037	1,4-Dichlorobenzene-d4	11.207

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	87
2			Nonanal	142	C9H18O	000124-19-6	86
3			Nonanal	142	C9H18O	000124-19-6	80
4			Nonanal	142	C9H18O	000124-19-6	80
5			Cyclohexanol, 2-methyl-, trans-	114	C7H14O	007443-52-9	46



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101823\
Data File : VV032464.D
Acq On : 18 Oct 2023 12:18
Operator : SY/MD
Sample : 04903-04
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AE7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.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...	1.101	5.6	ug/L	258842	1	5.667	231577	5.0
Acetamide, 2-fl...	1.455	1.7	ug/L	79869	1	5.667	231577	5.0
4-Chloro-1-butanol	1.728	0.9	ug/L	42191	1	5.667	231577	5.0
Pentanal	6.419	0.9	ug/L	43557	1	5.667	231577	5.0
Hexanal	8.259	1.6	ug/L	114109	2	8.847	352960	5.0
Heptanal	9.783	1.6	ug/L	114418	2	8.847	352960	5.0
Hexanal, 2-ethyl-	10.471	0.7	ug/L	51578	3	11.207	348172	5.0
Octanal	11.107	1.5	ug/L	104319	3	11.207	348172	5.0
1-Hexanol, 2-et...	11.496	2.5	ug/L	175920	3	11.207	348172	5.0
Nonanal	12.294	1.4	ug/L	96037	3	11.207	348172	5.0