

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
 Data File : VV032445.D
 Acq On : 17 Oct 2023 15:05
 Operator : SY/MD
 Sample : 04903-02
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AE5

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: VV032445.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.085	8	14	31	rVB2	98906	108950	20.13%	2.442%
2	1.156	31	36	42	rVB	13739	13056	2.41%	0.293%
3	1.192	42	47	52	rBV	7179	6395	1.18%	0.143%
4	1.275	64	73	90	rBV2	83665	120051	22.18%	2.691%
5	1.359	92	99	107	rBV	25707	38386	7.09%	0.861%
6	1.532	146	153	164	rVV	48959	62167	11.49%	1.394%
7	1.600	167	174	182	rVB4	6207	8315	1.54%	0.186%
8	1.729	206	214	220	rBV	13473	17393	3.21%	0.390%
9	1.767	220	226	233	rVB4	5780	7822	1.45%	0.175%
10	2.060	307	317	331	rBV	81885	123026	22.73%	2.758%
11	2.147	334	344	353	rBV	11652	29232	5.40%	0.655%
12	2.243	368	374	386	rVB	10832	16529	3.05%	0.371%
13	2.892	564	576	591	rBV4	7846	17438	3.22%	0.391%
14	3.600	777	796	815	rBV7	12226	44386	8.20%	0.995%
15	3.822	852	865	894	rBV2	53540	214367	39.61%	4.806%
16	4.256	983	1000	1024	rBV3	62851	179644	33.20%	4.027%
17	4.963	1203	1220	1241	rBV2	134267	353718	65.36%	7.930%
18	5.539	1386	1399	1416	rBV	118192	254034	46.94%	5.695%
19	5.841	1483	1493	1508	rVB10	5269	13208	2.44%	0.296%
20	5.995	1525	1541	1553	rBV2	79870	172279	31.83%	3.862%
21	6.233	1607	1615	1624	rBV3	4810	10301	1.90%	0.231%
22	6.921	1813	1829	1852	rBV2	35369	78859	14.57%	1.768%
23	7.249	1918	1931	1952	rBV	144564	280942	51.91%	6.298%
24	7.561	2019	2028	2045	rBV	22195	46962	8.68%	1.053%
25	7.879	2113	2127	2131	rBV6	15063	27117	5.01%	0.608%
26	8.031	2162	2174	2206	rBV	247060	541171	100.00%	12.132%
27	8.185	2214	2222	2244	rVB3	18904	43214	7.99%	0.969%
28	8.789	2398	2410	2428	rBV	199068	344888	63.73%	7.732%
29	8.953	2450	2461	2469	rBV4	5224	10403	1.92%	0.233%
30	9.082	2491	2501	2512	rVB2	14600	24958	4.61%	0.560%
31	9.336	2573	2580	2588	rBV5	4863	8822	1.63%	0.198%
32	9.487	2619	2627	2638	rVB4	4935	9041	1.67%	0.203%
33	9.551	2640	2647	2656	rVB3	4728	7761	1.43%	0.174%
34	9.664	2674	2682	2692	rVB3	5251	9719	1.80%	0.218%
35	9.757	2703	2711	2724	rBV8	11814	20797	3.84%	0.466%
36	10.159	2823	2836	2852	rVB	76465	126948	23.46%	2.846%

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37	10.297	2863	2879	2881	rBV6	4737	7984	1.48%	0.179%
38	10.329	2881	2889	2898	rVB2	15754	26779	4.95%	0.600%
39	10.391	2900	2908	2912	rBV4	6578	8991	1.66%	0.202%
40	10.452	2922	2927	2933	rBV6	4629	7577	1.40%	0.170%
41	10.481	2934	2936	2943	rVB4	6967	6833	1.26%	0.153%
42	10.680	2988	2998	3007	rBV4	5018	10442	1.93%	0.234%
43	10.857	3044	3053	3062	rBV2	20740	33079	6.11%	0.742%
44	10.992	3088	3095	3101	rBV7	3852	6268	1.16%	0.141%
45	11.098	3119	3128	3143	rBV5	13160	25454	4.70%	0.571%
46	11.188	3146	3156	3175	rVB	210627	337634	62.39%	7.569%
47	11.493	3238	3251	3257	rBV4	16861	36498	6.74%	0.818%
48	11.564	3264	3273	3292	rVB	179854	300660	55.56%	6.740%
49	11.857	3355	3364	3368	rBV2	7147	10655	1.97%	0.239%
50	11.960	3387	3396	3411	rVB3	9830	18069	3.34%	0.405%
51	12.056	3419	3426	3432	rBV3	5819	8533	1.58%	0.191%
52	12.194	3459	3469	3480	rBV2	10949	20239	3.74%	0.454%
53	12.294	3489	3500	3512	rBV4	19192	35287	6.52%	0.791%
54	12.358	3513	3520	3529	rVV2	7227	11271	2.08%	0.253%
55	12.410	3529	3536	3543	rVB2	7732	11512	2.13%	0.258%
56	12.673	3609	3618	3633	rBV2	6745	13618	2.52%	0.305%
57	12.825	3648	3665	3677	rBV6	9466	23154	4.28%	0.519%
58	13.107	3746	3753	3760	rVB9	3964	5851	1.08%	0.131%
59	13.162	3760	3770	3778	rBV7	4636	7909	1.46%	0.177%
60	13.214	3778	3786	3791	rBV8	6697	9687	1.79%	0.217%
61	13.275	3799	3805	3812	rBV7	3960	5458	1.01%	0.122%
62	13.384	3833	3839	3852	rVB9	3833	6009	1.11%	0.135%
63	13.699	3930	3937	3946	rVB9	3088	5934	1.10%	0.133%
64	13.988	4020	4027	4036	rVB2	4957	7397	1.37%	0.166%
65	14.387	4146	4151	4163	rBV2	4583	7635	1.41%	0.171%
66	15.056	4352	4359	4370	rVB10	7785	12178	2.25%	0.273%
67	16.127	4683	4692	4703	rVB8	11115	17917	3.31%	0.402%
68	16.255	4724	4732	4740	rVB9	4130	5619	1.04%	0.126%
69	17.046	4970	4978	4991	rBV	9537	16191	2.99%	0.363%

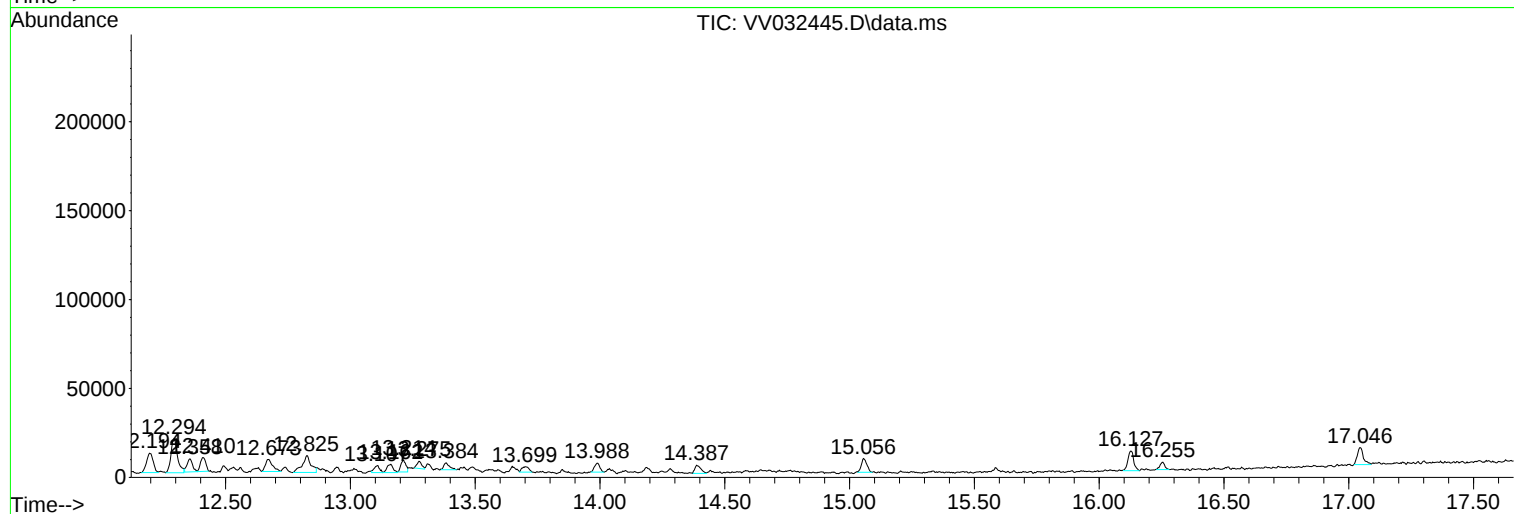
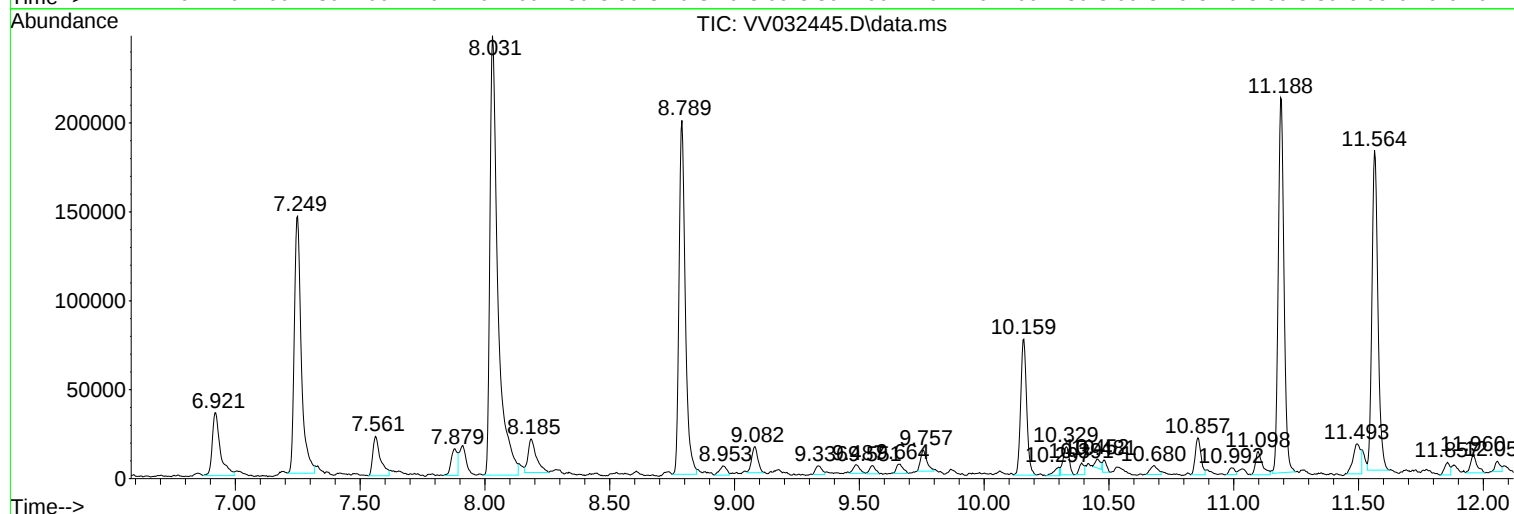
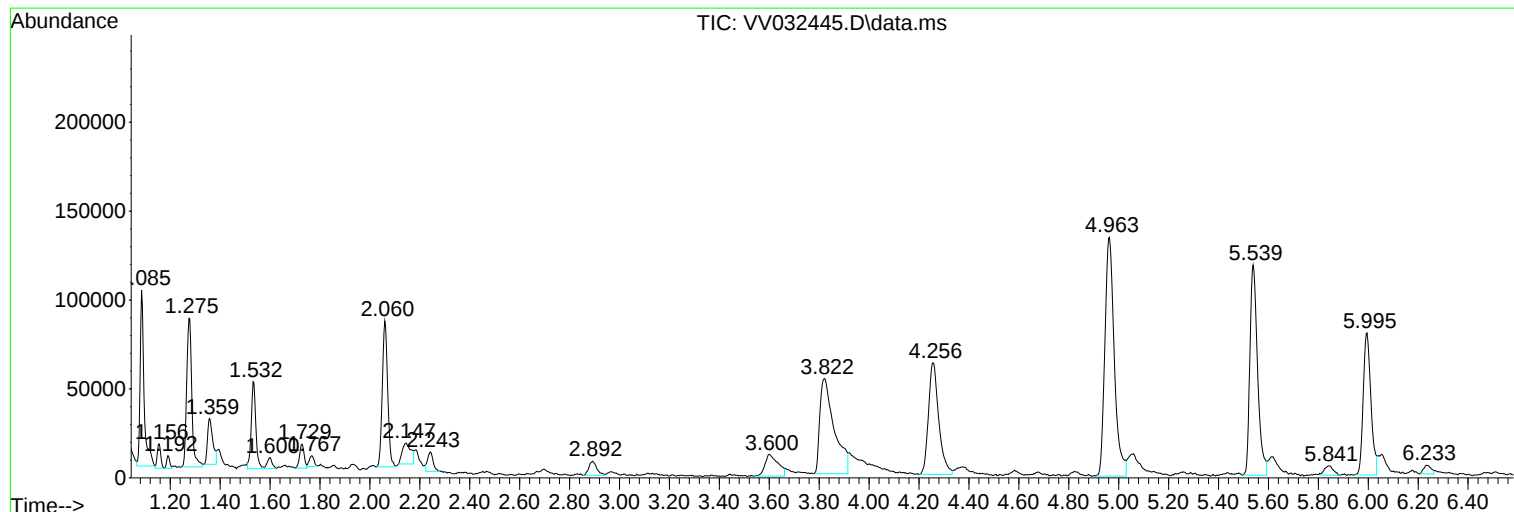
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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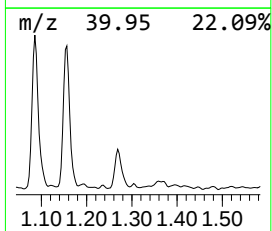
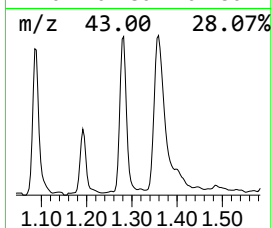
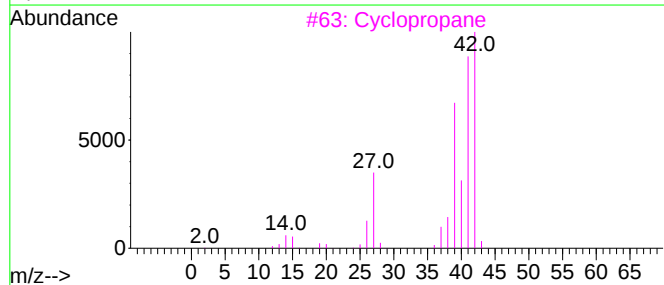
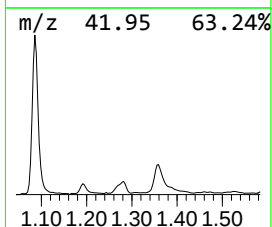
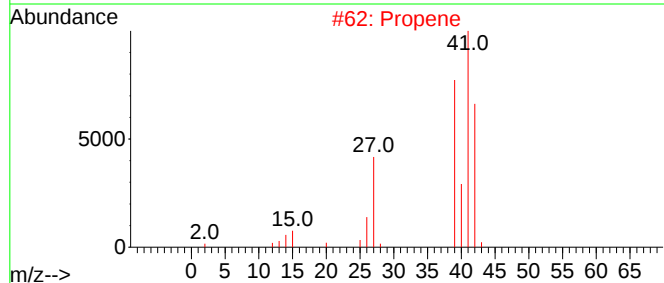
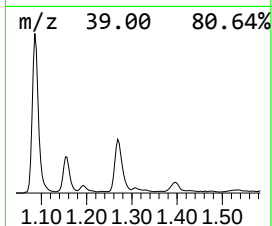
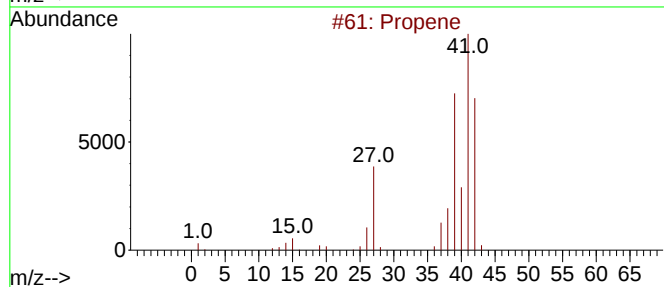
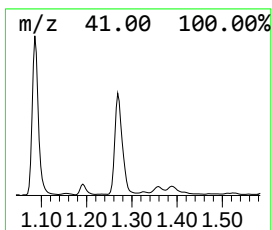
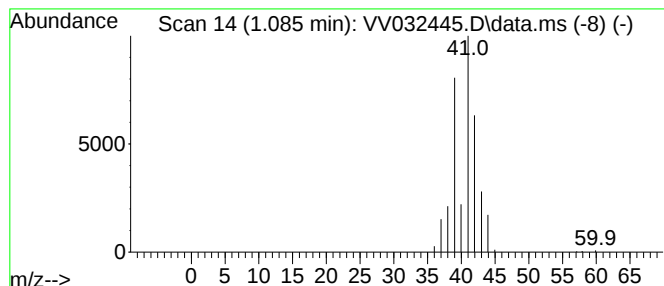
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.085	2.14 ug/L	108950	1,4-Difluorobenzene	5.539

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	40
4			Cyclopropane	42	C3H6	000075-19-4	9
5			Cyclopropene	40	C3H4	002781-85-3	9



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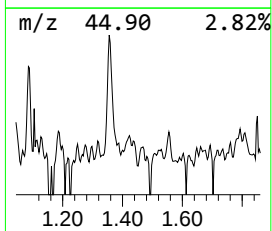
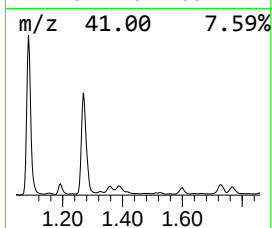
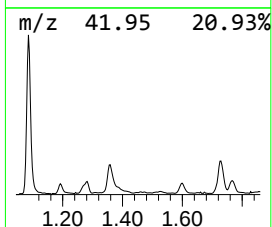
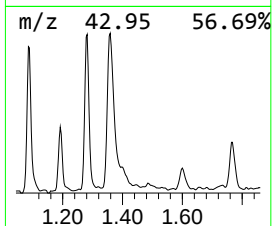
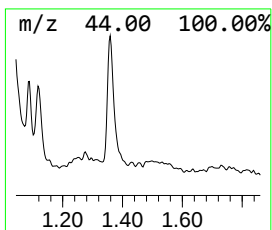
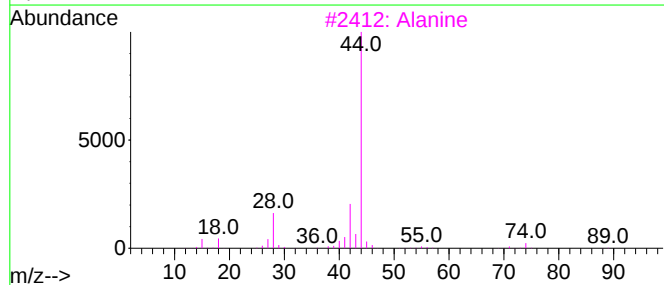
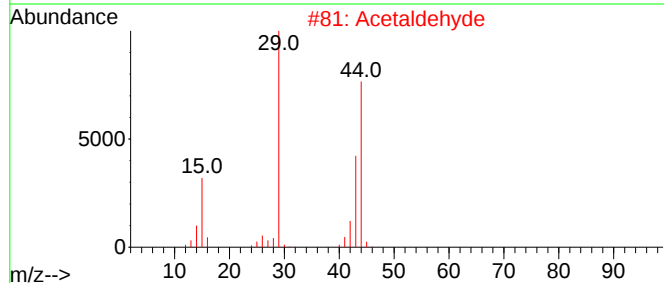
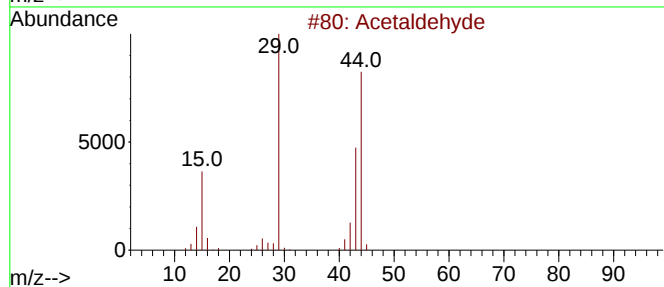
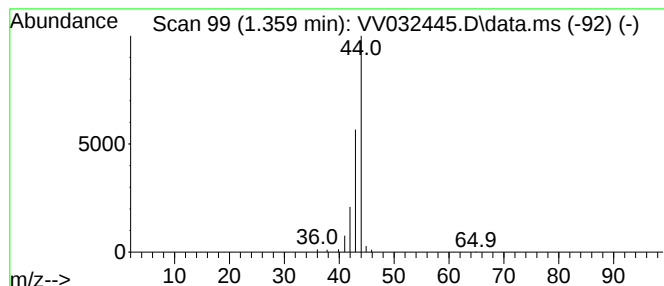
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	0.76 ug/L	38386	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	9
2			Acetaldehyde	44	C2H4O	000075-07-0	9
3			Alanine	89	C3H7NO2	000056-41-7	9
4			Ethylene oxide	44	C2H4O	000075-21-8	7
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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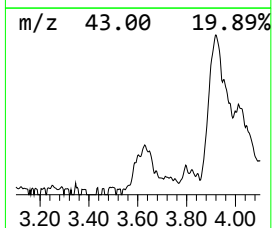
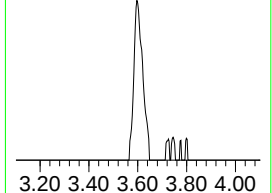
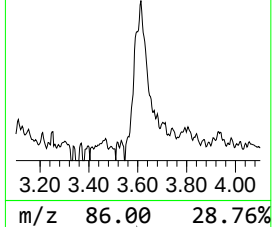
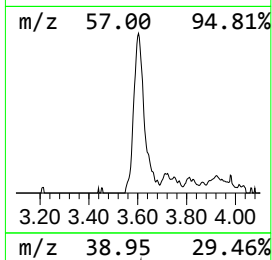
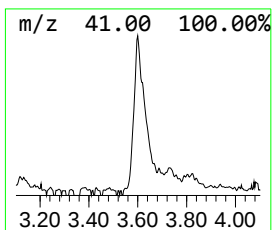
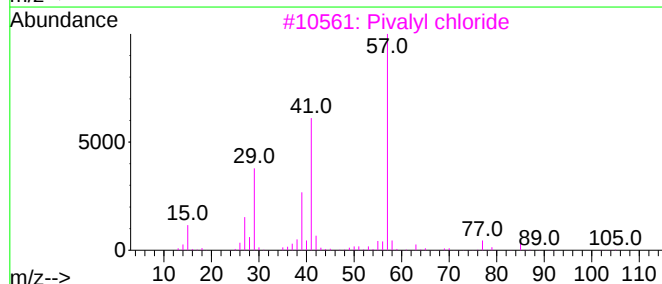
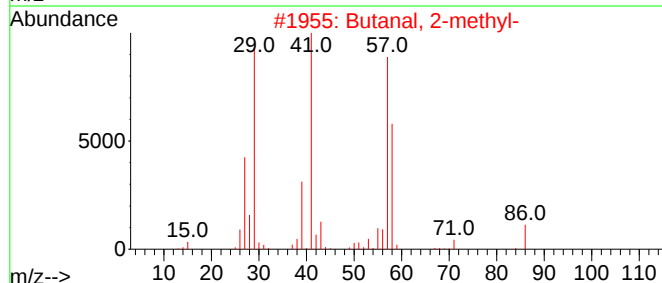
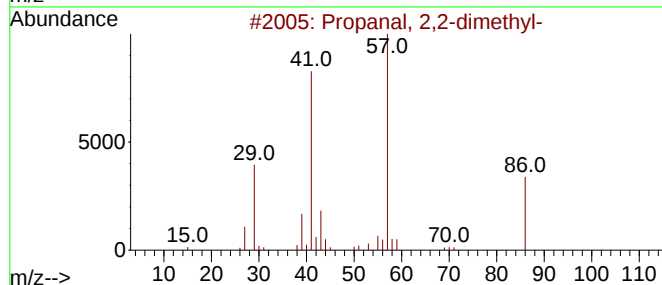
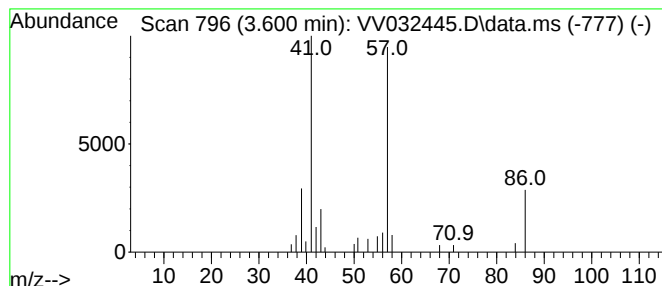
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Propanal, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.600	0.87 ug/L	44386	1,4-Difluorobenzene	5.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2			Butanal, 2-methyl-	86	C5H10O	000096-17-3	45
3			Pivalyl chloride	120	C5H9ClO	003282-30-2	40
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	33
5			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	28



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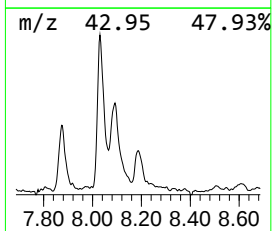
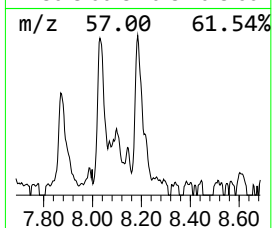
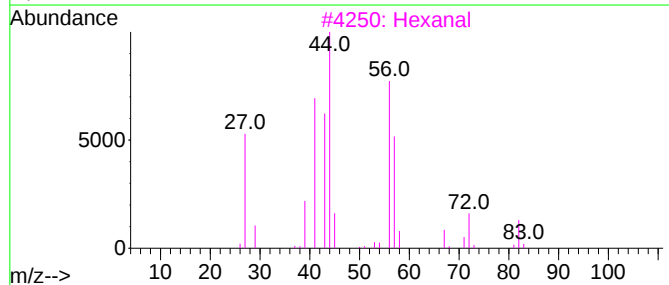
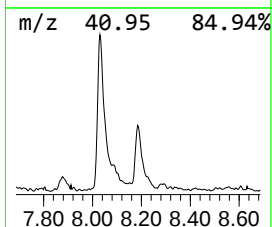
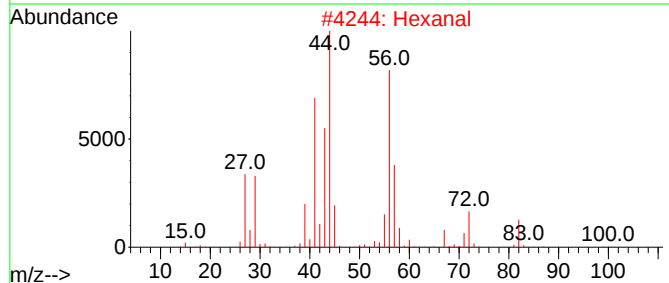
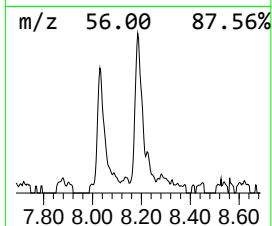
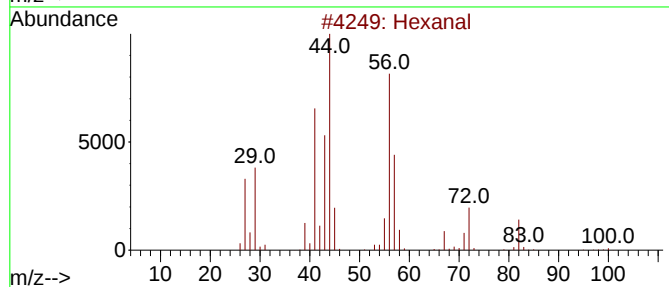
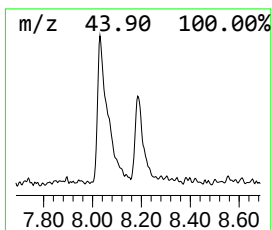
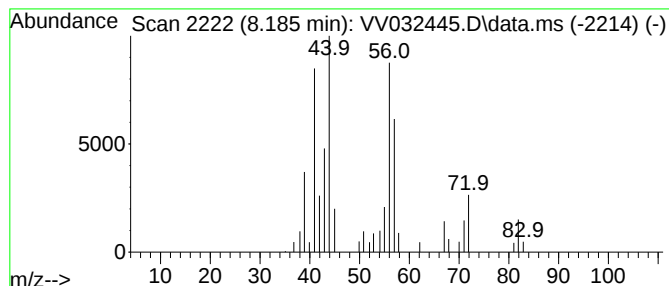
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.185	0.63 ug/L	43214	Chlorobenzene-d5	8.789

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	83
2	Hexanal			100	C6H12O	000066-25-1	72
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	59
5	Cyclobutanol, 2-ethyl-			100	C6H12O	035301-43-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032445.D
Acq On : 17 Oct 2023 15:05
Operator : SY/MD
Sample : 04903-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AE5

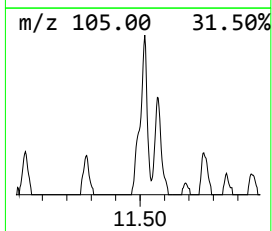
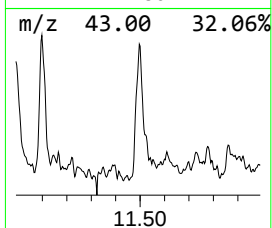
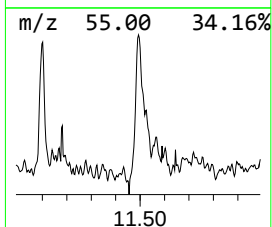
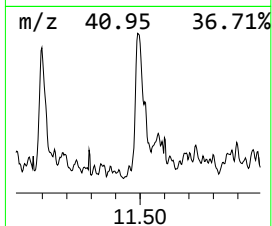
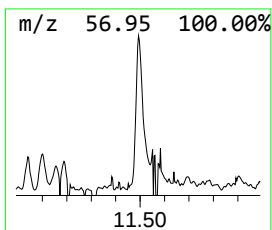
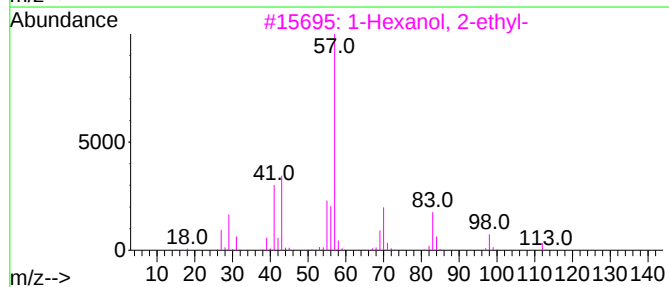
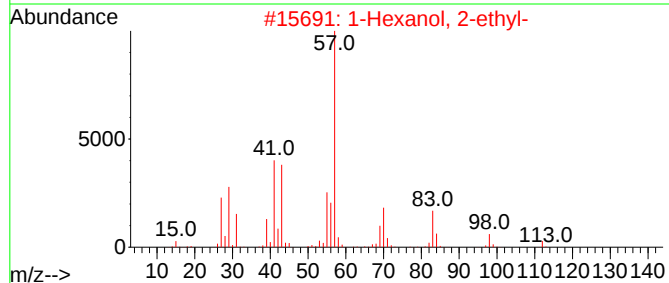
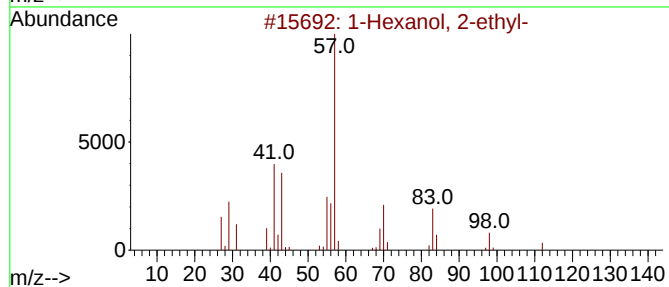
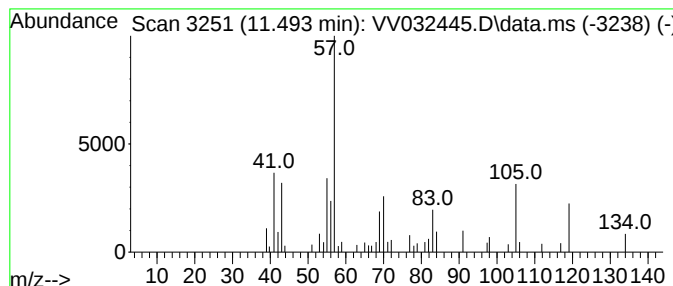
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.493	0.54 ug/L	36498	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	50
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	47
5			2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032445.D
Acq On : 17 Oct 2023 15:05
Operator : SY/MD
Sample : 04903-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AE5

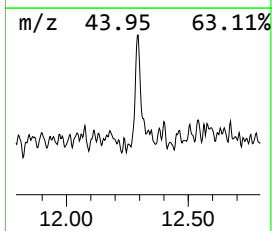
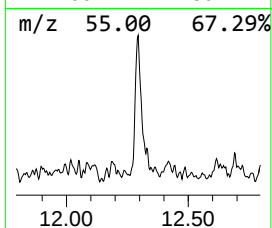
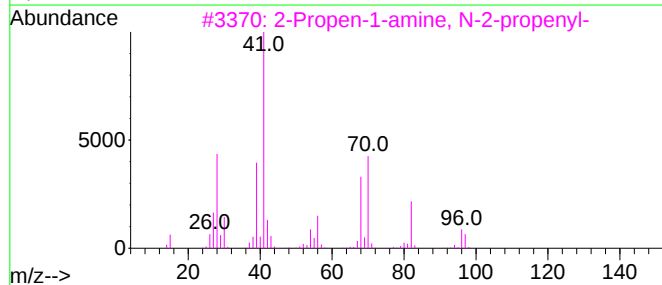
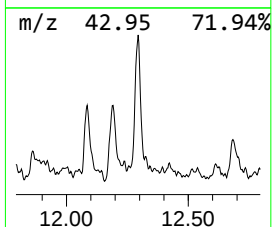
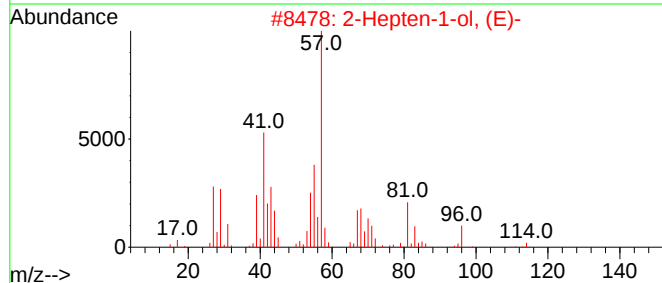
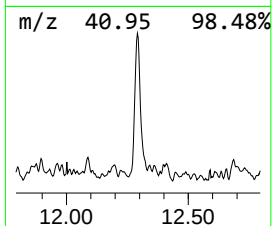
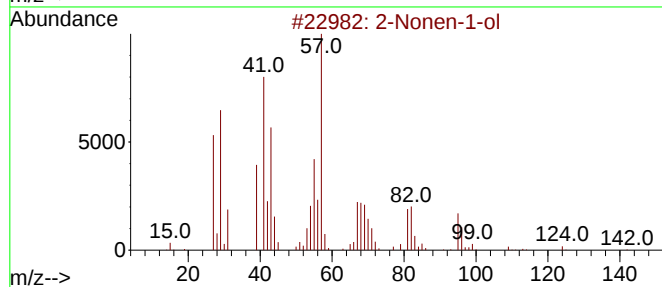
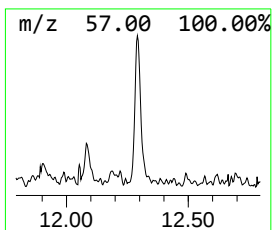
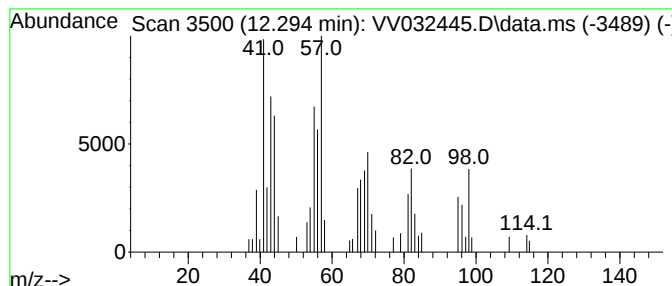
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 unknown-02 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.294	0.52 ug/L	35287	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonen-1-ol			142	C9H18O	022104-79-6	35
2	2-Hepten-1-ol, (E)-			114	C7H14O	033467-76-4	30
3	2-Propen-1-amine, N-2-propenyl-			97	C6H11N	000124-02-7	25
4	2-Propen-1-amine, N-2-propenyl-			97	C6H11N	000124-02-7	25
5	Aziridine, 2-ethyl-			71	C4H9N	002549-67-9	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032445.D
Acq On : 17 Oct 2023 15:05
Operator : SY/MD
Sample : 04903-02
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AE5

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...	1.085	2.1	ug/L	108950	1	5.539	254034	5.0
unknown-01	1.359	0.8	ug/L	38386	1	5.539	254034	5.0
Propanal, 2,2-d...	3.600	0.9	ug/L	44386	1	5.539	254034	5.0
Hexanal	8.185	0.6	ug/L	43214	2	8.789	344888	5.0
1-Hexanol, 2-et...	11.493	0.5	ug/L	36498	3	11.191	337634	5.0
unknown-02	12.294	0.5	ug/L	35287	3	11.191	337634	5.0