

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
 Data File : VV027699.D
 Acq On : 02 Sep 2022 05:05
 Operator : SY/MD
 Sample : N4402-13
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBVC6

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\SFAMVTR083122WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV027699.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	74	83	97	rBV2	118088	138426	21.49%	2.097%
2	1.568	157	164	176	rVB	84722	96971	15.05%	1.469%
3	1.806	233	238	245	rVB2	8958	10742	1.67%	0.163%
4	2.034	300	309	317	rBV8	4898	10874	1.69%	0.165%
5	2.108	321	332	346	rVB	175133	254210	39.46%	3.850%
6	3.908	878	892	919	rBV2	113161	328647	51.02%	4.978%
7	4.346	1011	1028	1060	rVB	117821	301221	46.76%	4.562%
8	5.043	1226	1245	1281	rBV2	250902	644169	100.00%	9.757%
9	5.616	1411	1423	1447	rBV	148814	312876	48.57%	4.739%
10	5.918	1507	1517	1535	rVB7	7954	17889	2.78%	0.271%
11	6.066	1550	1563	1583	rBV	142980	302543	46.97%	4.582%
12	6.985	1839	1849	1865	rBV	54160	102596	15.93%	1.554%
13	7.313	1940	1951	1969	rBV	271332	483827	75.11%	7.328%
14	7.394	1970	1976	1986	rVB4	6597	12974	2.01%	0.197%
15	7.625	2037	2048	2070	rBV	30103	58751	9.12%	0.890%
16	7.976	2147	2157	2172	rVB3	14490	26104	4.05%	0.395%
17	8.092	2180	2193	2212	rBV	166542	403783	62.68%	6.116%
18	8.185	2213	2222	2237	rVB2	201157	370347	57.49%	5.609%
19	8.317	2250	2263	2291	rVB	204263	396076	61.49%	5.999%
20	8.850	2413	2429	2454	rBV	233732	401089	62.26%	6.075%
21	9.018	2471	2481	2487	rBV2	8457	12708	1.97%	0.192%
22	9.069	2490	2497	2505	rVV7	5136	8185	1.27%	0.124%
23	9.140	2508	2519	2537	rBV	108442	175394	27.23%	2.657%
24	9.262	2547	2557	2572	rVB2	30446	53501	8.31%	0.810%
25	9.548	2637	2646	2656	rBV5	5504	9816	1.52%	0.149%
26	9.702	2682	2694	2704	rBV8	5788	9866	1.53%	0.149%
27	10.214	2842	2853	2869	rBV	91244	150377	23.34%	2.278%
28	10.294	2869	2878	2891	rVB4	11873	19406	3.01%	0.294%
29	10.522	2940	2949	2950	rBV7	5476	6449	1.00%	0.098%
30	10.815	3029	3040	3051	rBV2	28543	45267	7.03%	0.686%
31	10.918	3062	3072	3083	rBV3	5089	7957	1.24%	0.121%
32	11.249	3163	3175	3180	rBV	215029	340146	52.80%	5.152%
33	11.281	3180	3185	3198	rVB	222980	347235	53.90%	5.259%
34	11.529	3249	3262	3280	rBV	51919	98177	15.24%	1.487%
35	11.622	3280	3291	3312	rVB	274602	451127	70.03%	6.833%
36	12.098	3428	3439	3441	rBV9	5570	8485	1.32%	0.129%

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.577	3575	3588	3603	rVB4	33799	74273	11.53%	1.125%
38	12.882	3673	3683	3687	rBV5	5691	8518	1.32%	0.129%
39	12.908	3687	3691	3701	rVB6	5371	7364	1.14%	0.112%
40	12.995	3708	3718	3728	rBV4	10500	18515	2.87%	0.280%
41	13.455	3848	3861	3870	rBV7	11398	18864	2.93%	0.286%
42	13.979	4014	4024	4036	rVB4	4743	7115	1.10%	0.108%
43	14.082	4048	4056	4071	rBV4	7094	14400	2.24%	0.218%
44	14.963	4321	4330	4333	rBV3	5614	7817	1.21%	0.118%
45	14.988	4333	4338	4348	rVB5	7694	11983	1.86%	0.181%
46	15.664	4540	4548	4555	rBV8	4707	6462	1.00%	0.098%
47	16.480	4794	4802	4812	rBV6	5761	8888	1.38%	0.135%

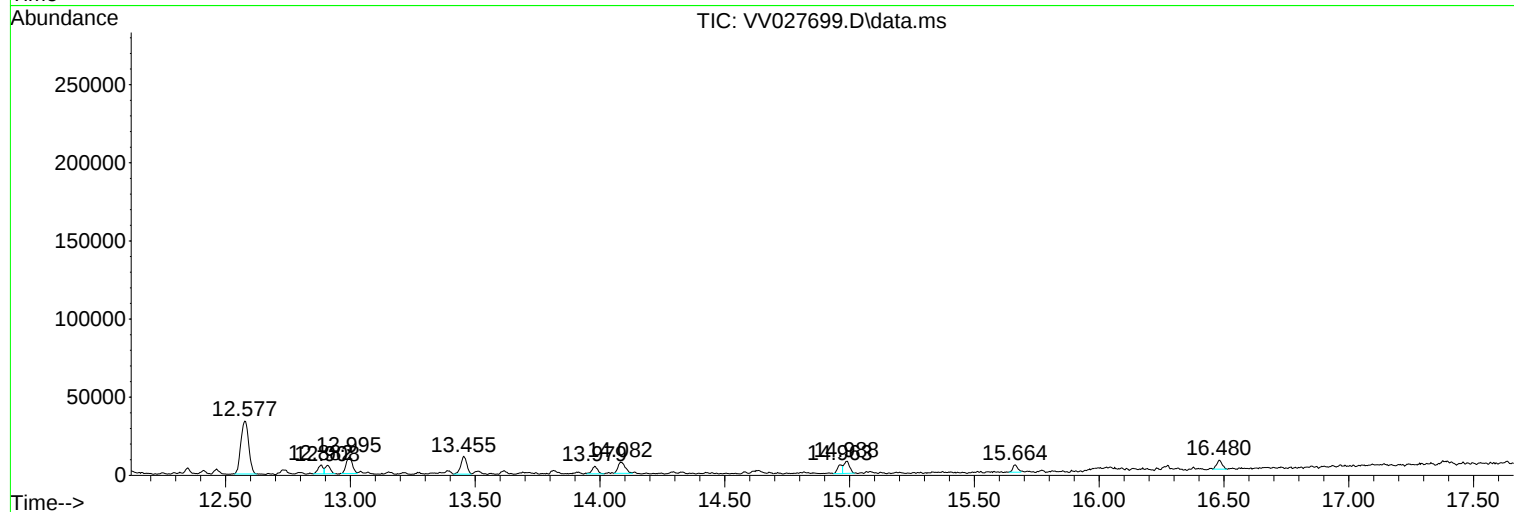
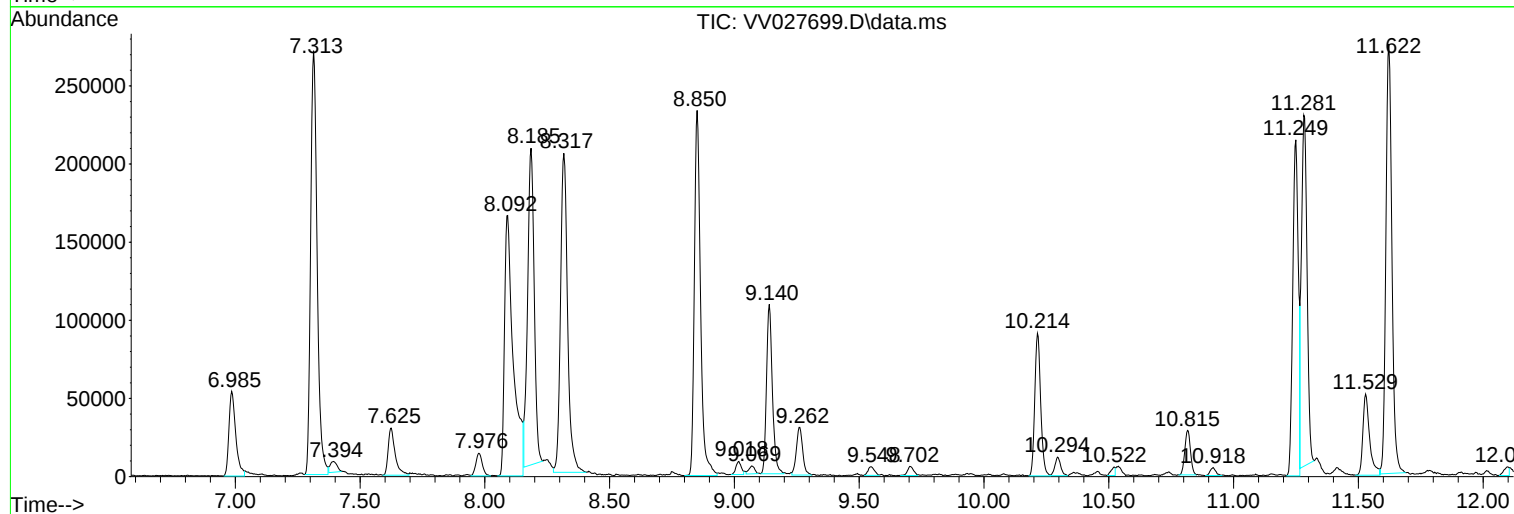
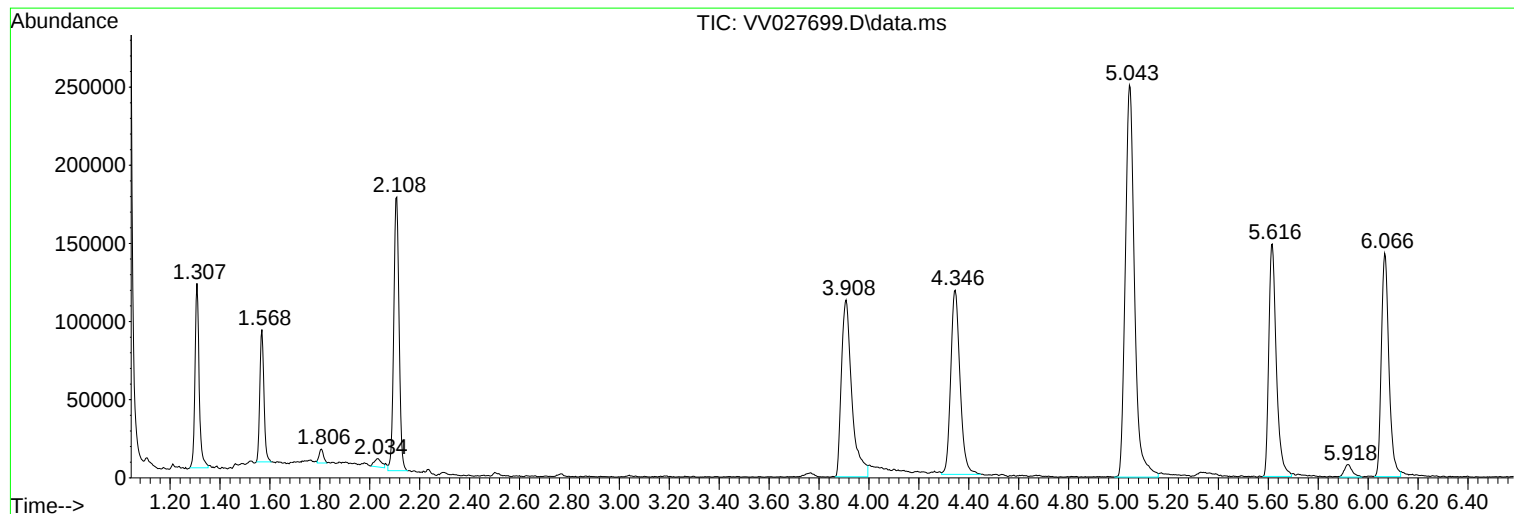
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Quant Title : TRACE VOA SFAM1.0

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



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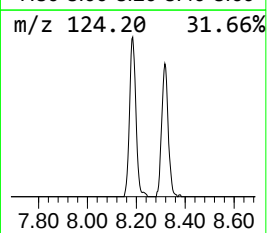
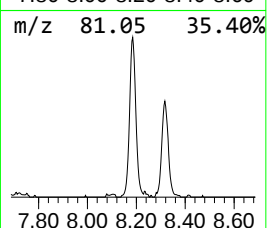
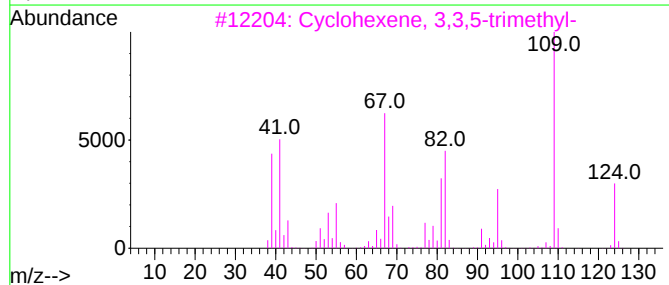
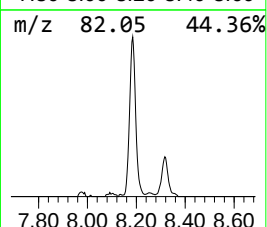
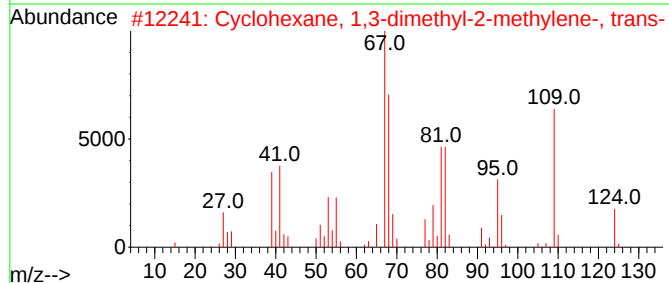
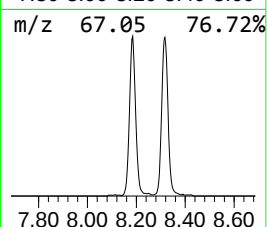
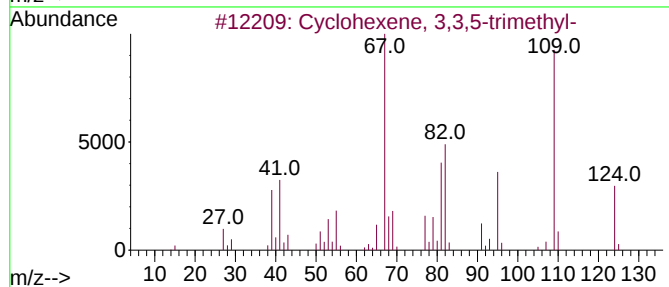
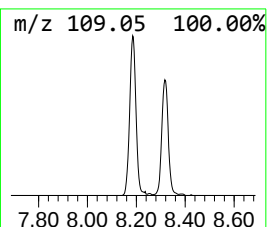
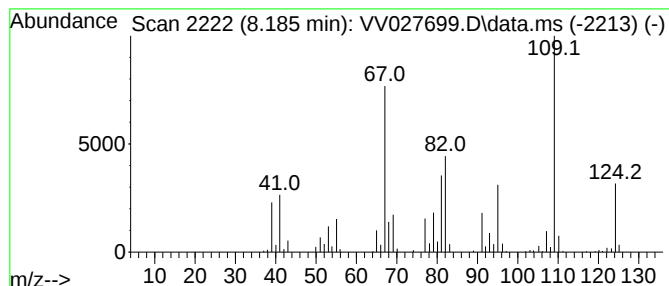
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Cyclohexene, 3,3,5-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.185	4.62 ug/L	370347	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	95
2			Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	020348-74-7	93
3			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	90
4			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	90
5			1,3-Hexadiene, 2,3,5-trimethyl-	124	C9H16	061142-34-5	70



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ALS Vial : 29 Sample Multiplier: 1

Instrument :
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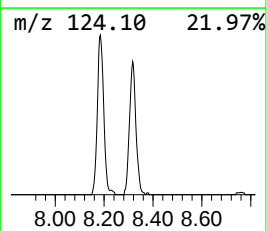
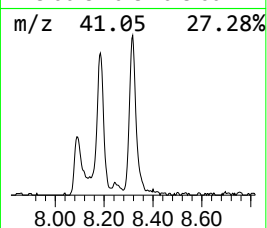
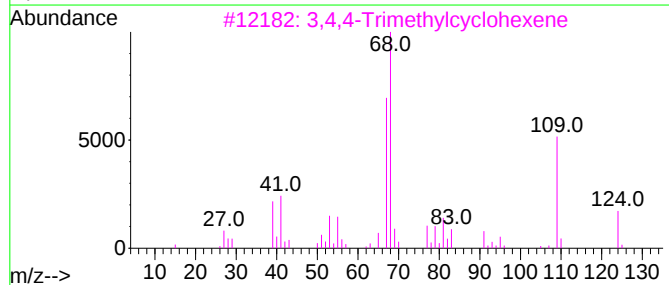
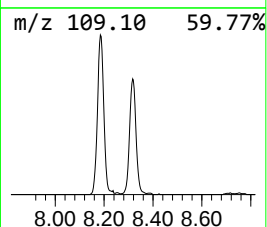
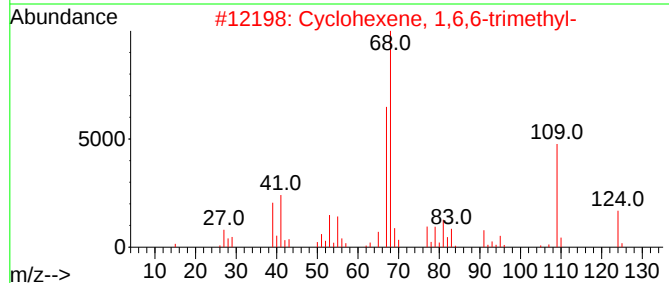
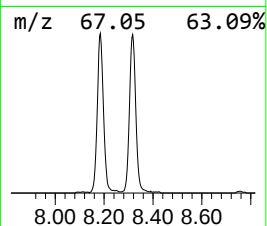
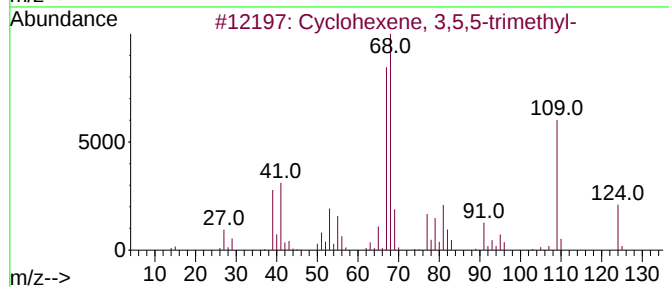
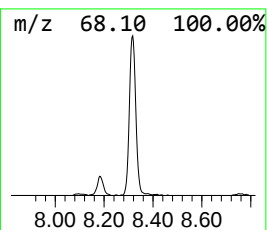
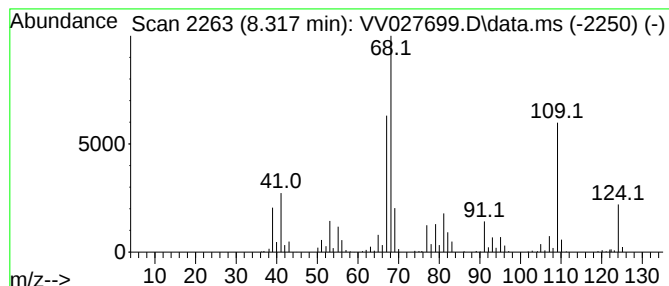
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Cyclohexene, 3,5,5-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.317	4.94 ug/L	396076	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	96
2			Cyclohexene, 1,6,6-trimethyl-	124	C9H16	069745-49-9	96
3			3,4,4-Trimethylcyclohexene	124	C9H16	1000113-50-1	95
4			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	94
5			1,3-Hexadiene, 2,3,5-trimethyl-	124	C9H16	061142-34-5	55



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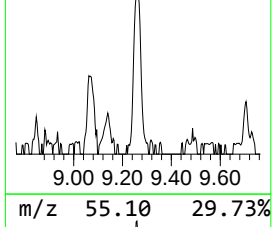
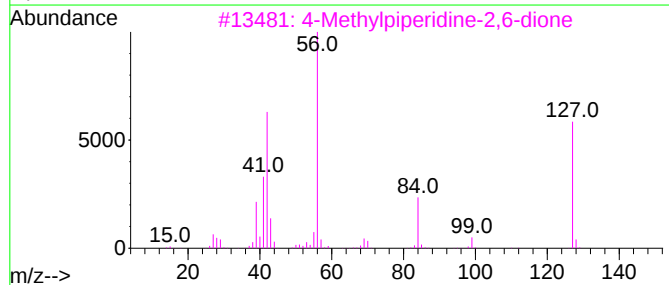
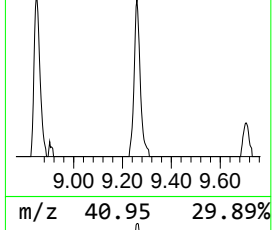
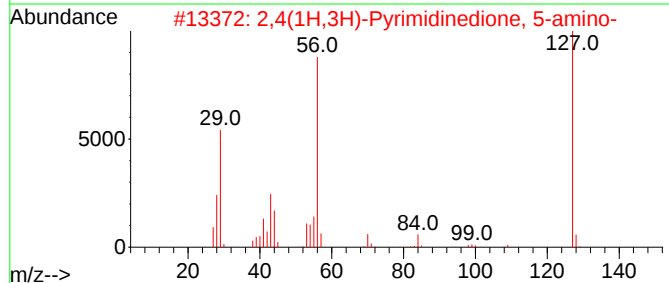
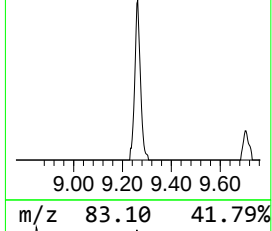
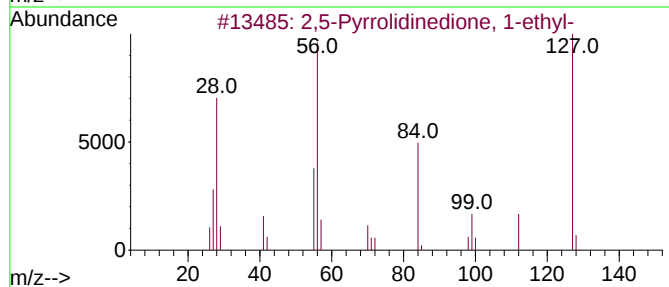
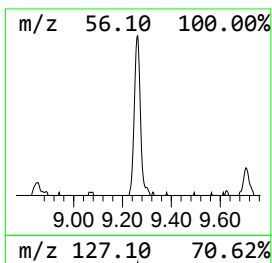
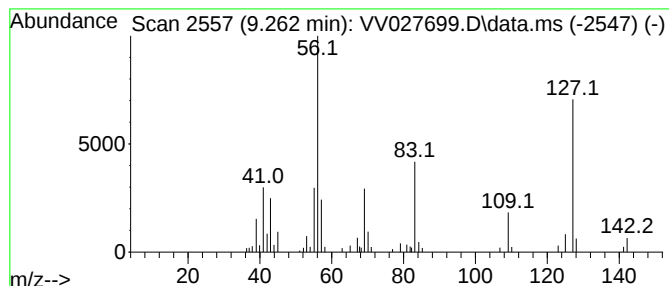
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2,5-Pyrrolidinedione, 1-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.262	0.67 ug/L	53501	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Pyrrolidinedione, 1-ethyl-	127	C6H9NO2	002314-78-5	52
2			2,4(1H,3H)-Pyrimidinedione, 5-am...	127	C4H5N3O2	000932-52-5	40
3			4-Methylpiperidine-2,6-dione	127	C6H9NO2	025077-26-3	38
4			2H-Pyran-2-one, tetrahydro-4,4,6...	142	C8H14O2	010603-06-2	37
5			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	35



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ALS Vial : 29 Sample Multiplier: 1

Instrument :
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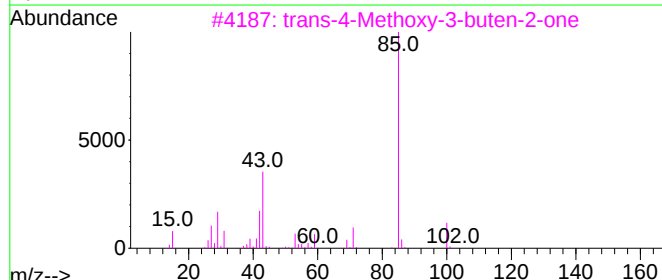
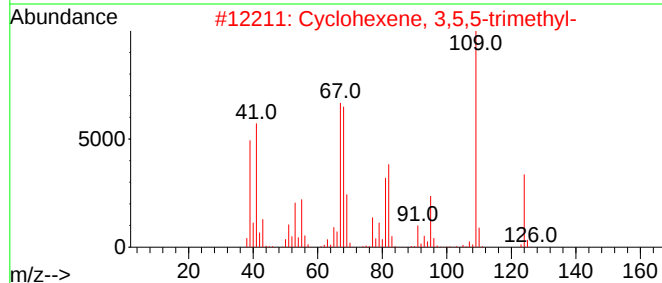
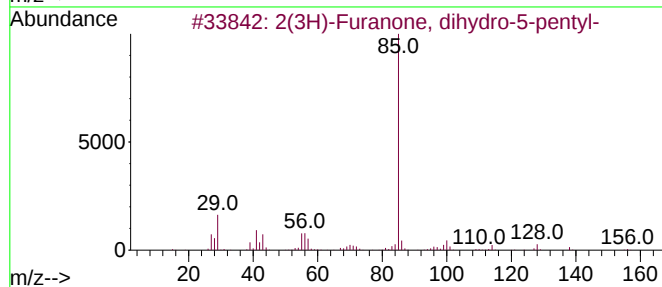
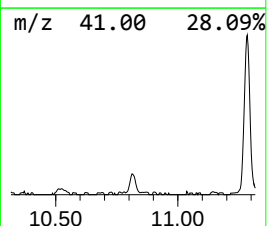
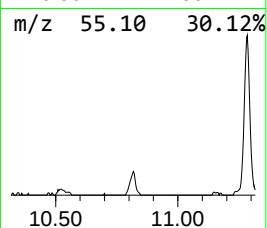
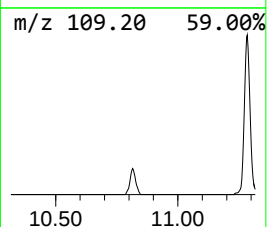
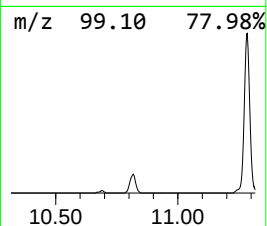
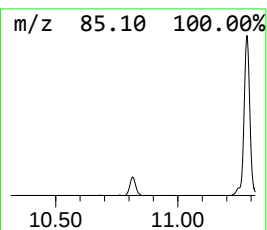
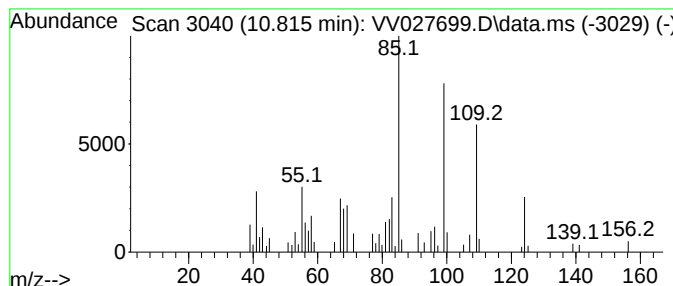
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.815	0.67 ug/L	45267	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	18		
2	Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	18		
3	trans-4-Methoxy-3-buten-2-one	100	C5H8O2	051731-17-0	18		
4	2,4-Heptadiene, 2,4-dimethyl-	124	C9H16	074421-05-9	15		
5	3-Heptyne, 2,2-dimethyl-	124	C9H16	029022-29-5	15		



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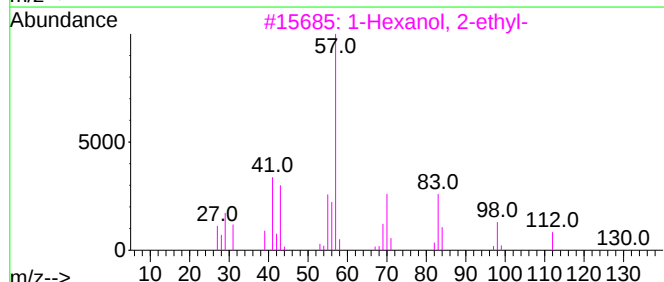
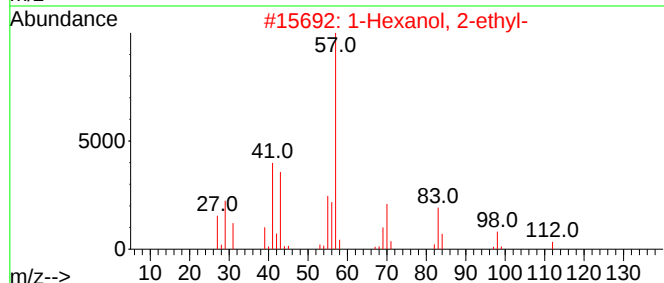
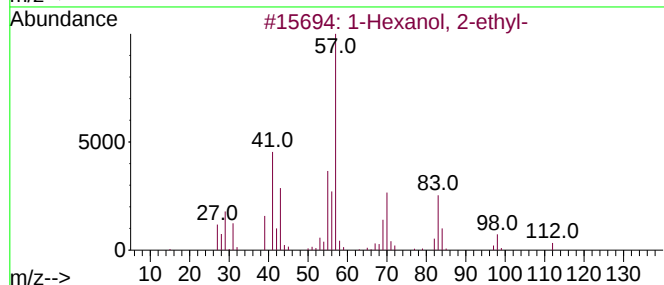
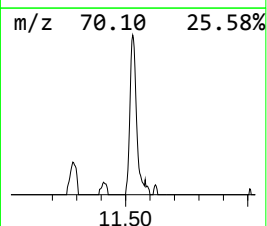
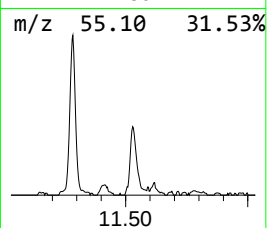
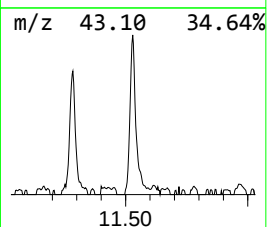
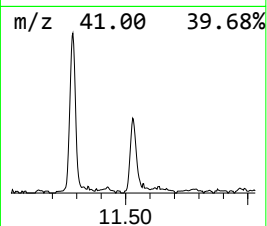
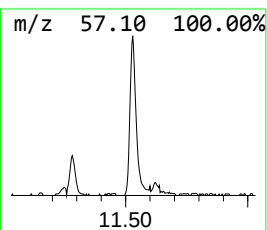
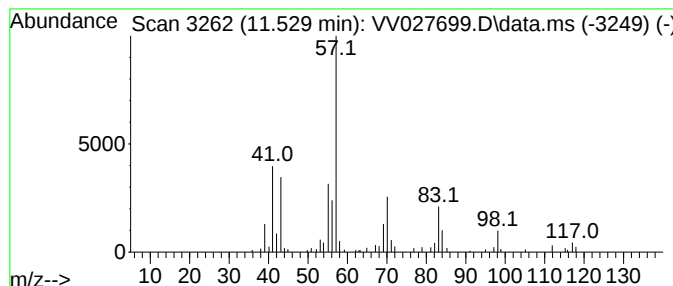
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	1.44 ug/L	98177	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027699.D
Acq On : 02 Sep 2022 05:05
Operator : SY/MD
Sample : N4402-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBVC6

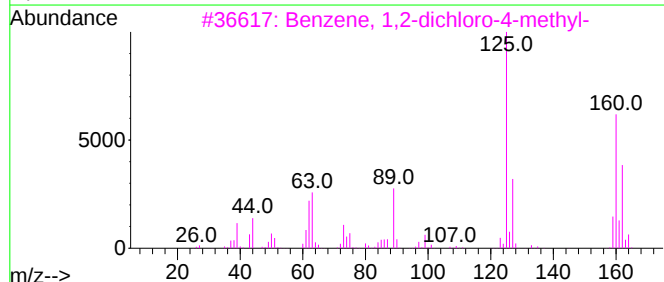
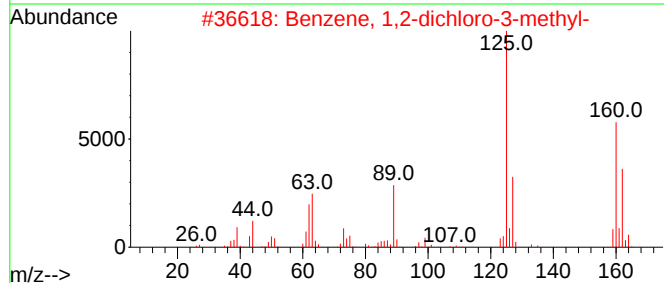
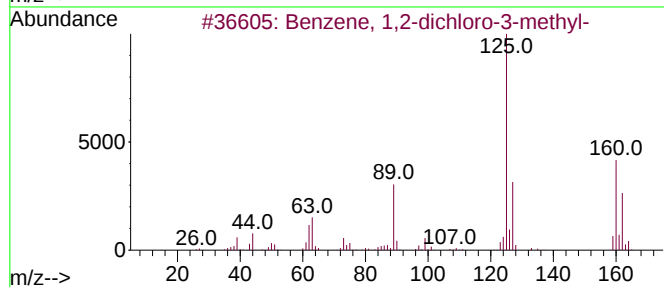
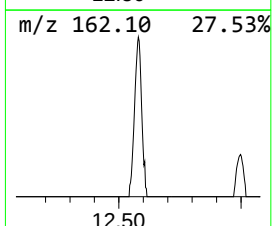
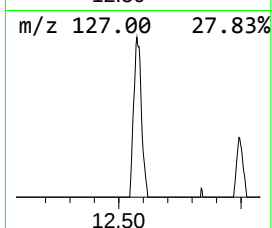
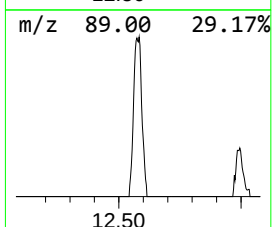
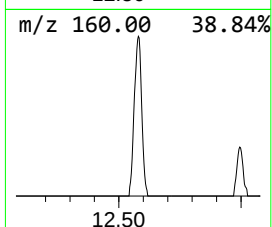
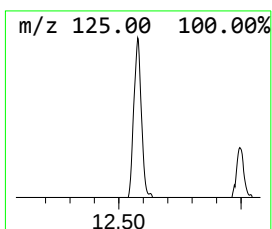
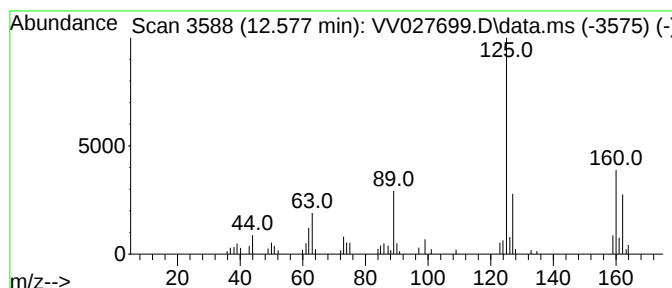
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Benzene, 1,2-dichloro-3-met... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.577	1.09 ug/L	74273	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	98
2			Benzene, 1,2-dichloro-3-methyl-	160	C7H6Cl2	032768-54-0	97
3			Benzene, 1,2-dichloro-4-methyl-	160	C7H6Cl2	000095-75-0	97
4			Benzene, 1,3-dichloro-2-methyl-	160	C7H6Cl2	000118-69-4	97
5			Benzene, 1,4-dichloro-2-methyl-	160	C7H6Cl2	019398-61-9	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027699.D
Acq On : 02 Sep 2022 05:05
Operator : SY/MD
Sample : N4402-13
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBVC6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.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
Cyclohexene, 3,...	8.185	4.6	ug/L	370347	2	8.850	401089	5.0
Cyclohexene, 3,...	8.317	4.9	ug/L	396076	2	8.850	401089	5.0
2,5-Pyrrolidine...	9.262	0.7	ug/L	53501	2	8.850	401089	5.0
unknown-01	10.815	0.7	ug/L	45267	3	11.249	340146	5.0
1-Hexanol, 2-et...	11.529	1.4	ug/L	98177	3	11.249	340146	5.0
Benzene, 1,2-di...	12.577	1.1	ug/L	74273	3	11.249	340146	5.0