

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
 Data File : VV027710.D
 Acq On : 02 Sep 2022 09:33
 Operator : SY/MD
 Sample : N4404-14
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBVC5

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: VV027710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.297	69	80	100	rBV2	87492	104833	15.90%	1.878%
2	1.561	153	162	176	rBV	79239	93989	14.25%	1.684%
3	1.796	226	235	240	rBV4	5106	7172	1.09%	0.128%
4	1.986	281	294	312	rBV	10825	38594	5.85%	0.691%
5	2.098	320	329	348	rVB2	170847	258357	39.18%	4.628%
6	2.201	353	361	372	rBV	15918	24108	3.66%	0.432%
7	2.285	381	387	400	rVB3	7354	13197	2.00%	0.236%
8	3.108	631	643	656	rBV4	29135	63355	9.61%	1.135%
9	3.908	875	892	897	rBV3	57502	139445	21.15%	2.498%
10	4.346	1012	1028	1053	rBV2	130364	367186	55.69%	6.577%
11	5.030	1224	1241	1261	rBV2	302031	659352	100.00%	11.811%
12	5.593	1405	1416	1432	rVB	171213	318390	48.29%	5.703%
13	5.879	1495	1505	1520	rVB3	66895	127574	19.35%	2.285%
14	6.046	1545	1557	1575	rVB	159968	322189	48.86%	5.771%
15	6.288	1618	1632	1643	rBV4	9085	17907	2.72%	0.321%
16	6.513	1692	1702	1715	rBV2	7491	14312	2.17%	0.256%
17	6.972	1834	1845	1862	rBV2	83353	148625	22.54%	2.662%
18	7.310	1929	1950	1966	rBV	277841	513779	77.92%	9.203%
19	7.628	2036	2049	2067	rVB	35290	62261	9.44%	1.115%
20	7.853	2109	2119	2128	rVB4	8662	14259	2.16%	0.255%
21	7.976	2143	2157	2176	rBV	222350	366399	55.57%	6.563%
22	8.117	2186	2201	2215	rBV	254949	477010	72.35%	8.545%
23	8.185	2217	2222	2240	rVB4	33757	62253	9.44%	1.115%
24	8.316	2254	2263	2283	rVB4	28372	57856	8.77%	1.036%
25	8.857	2420	2431	2452	rBV	205815	342069	51.88%	6.128%
26	8.979	2459	2469	2483	rVB3	26502	43730	6.63%	0.783%
27	9.146	2511	2521	2532	rBV	9437	15585	2.36%	0.279%
28	9.734	2692	2704	2716	rBV2	12438	20848	3.16%	0.373%
29	10.217	2842	2854	2867	rBV	93736	147720	22.40%	2.646%
30	11.249	3163	3175	3196	rBV	187485	303509	46.03%	5.437%
31	11.532	3254	3263	3277	rBV2	28822	48623	7.37%	0.871%
32	11.622	3280	3291	3309	rVB	236908	374425	56.79%	6.707%
33	12.345	3505	3516	3531	rVB5	8618	13595	2.06%	0.244%

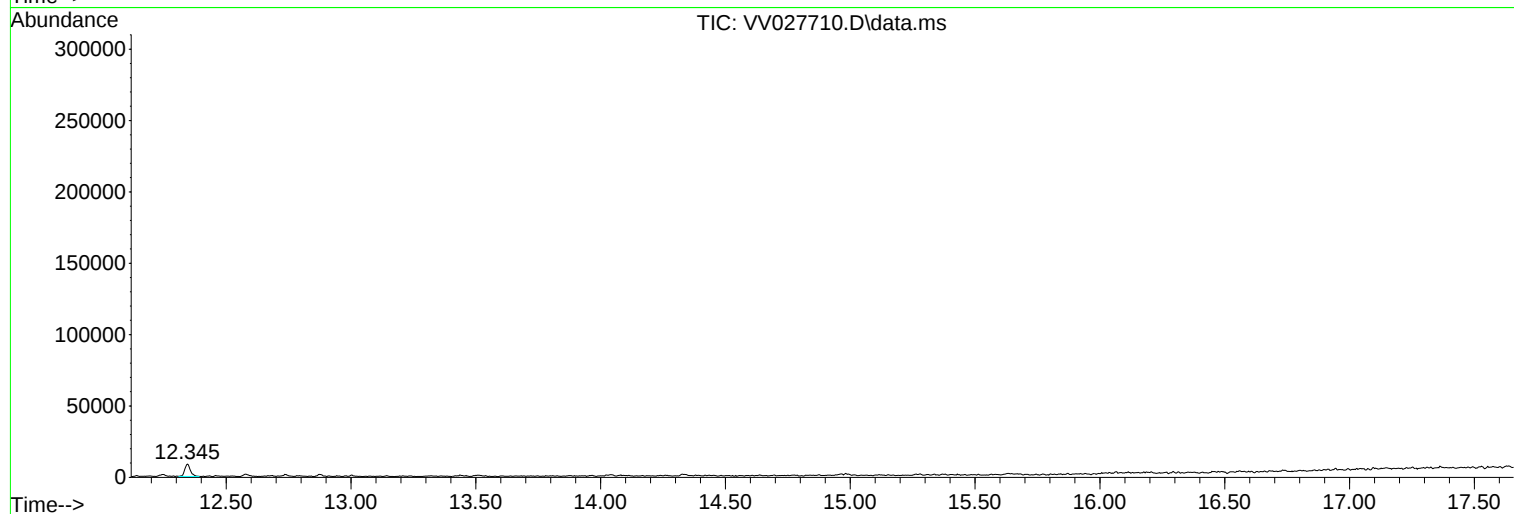
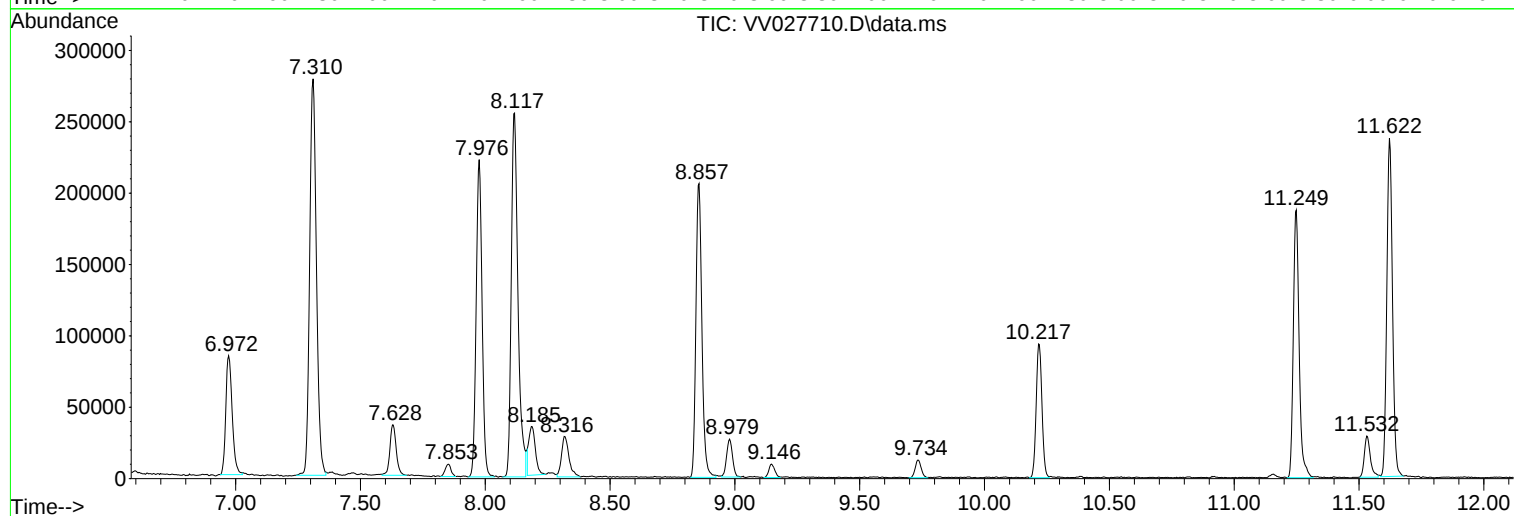
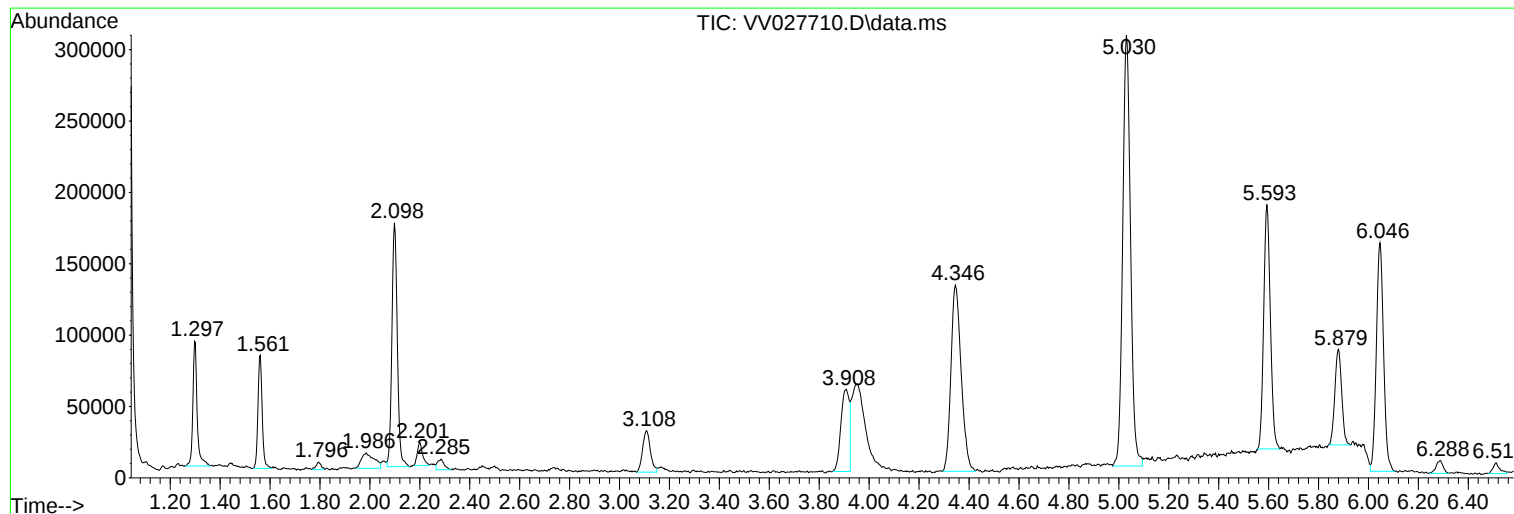
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Quant Title : TRACE VOA SFAM1.0

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



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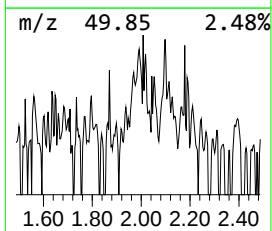
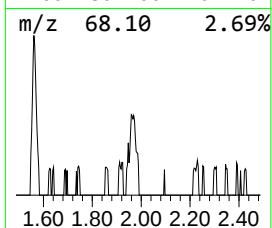
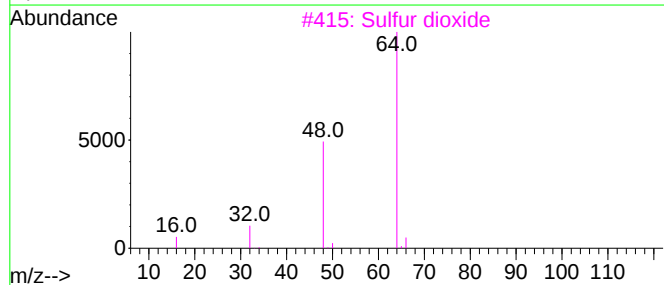
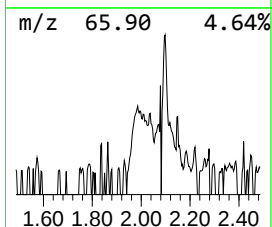
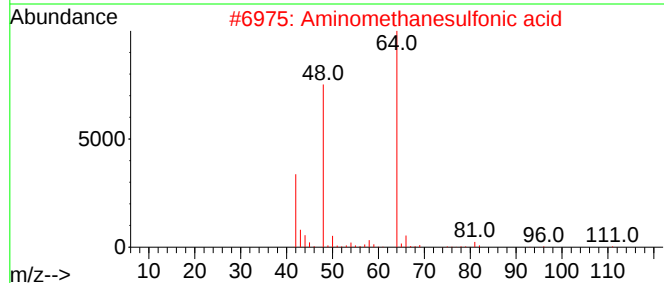
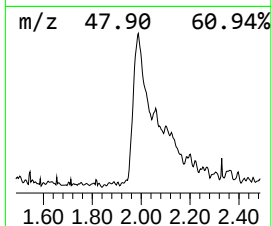
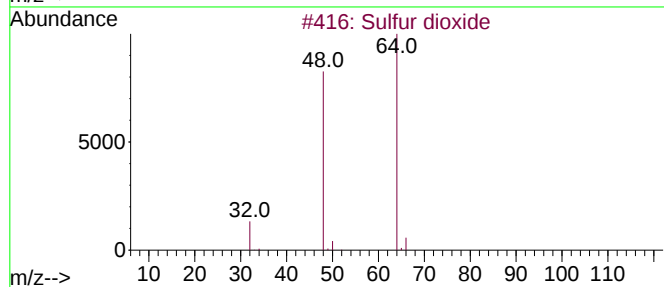
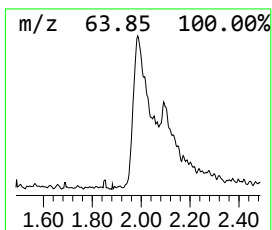
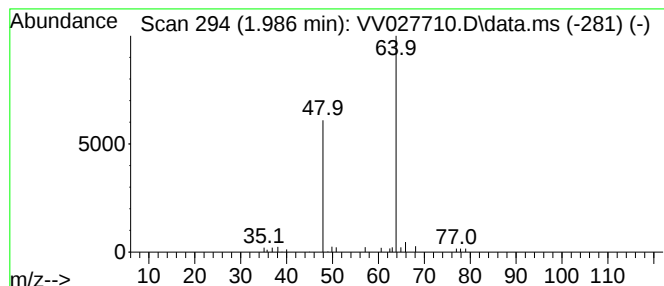
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.986	0.61 ug/L	38594	1,4-Difluorobenzene	5.593

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Sulfur dioxide	64	O2S	007446-09-5	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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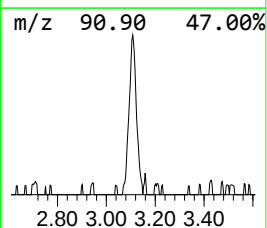
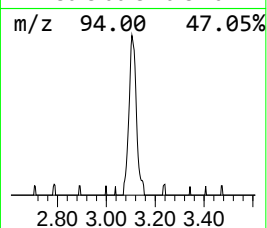
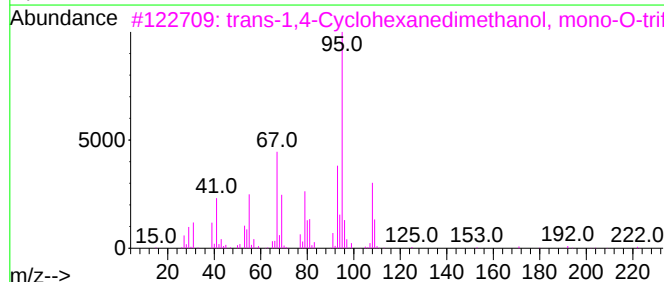
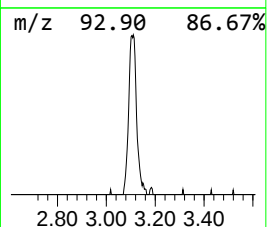
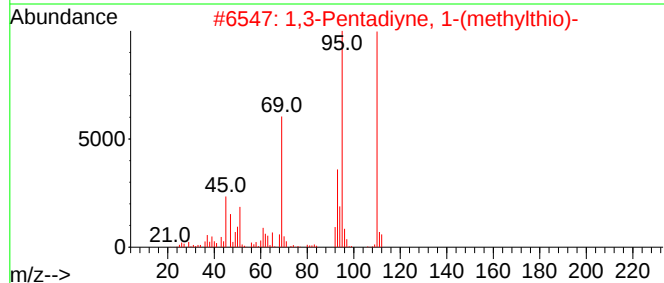
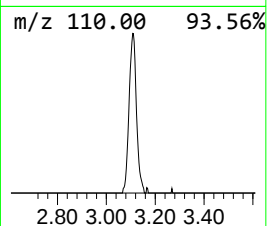
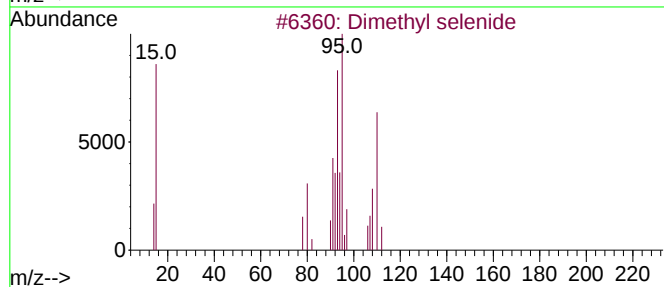
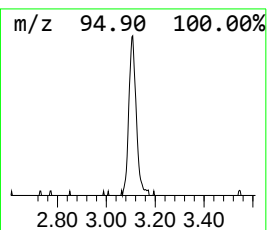
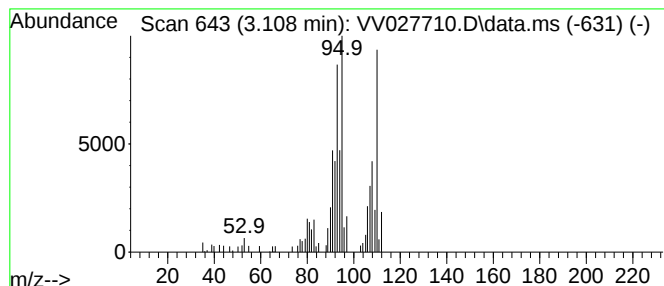
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR083122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Dimethyl selenide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.108	0.99 ug/L	63355	1,4-Difluorobenzene	5.593

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl selenide	110	C2H6Se	000593-79-3	87
2			1,3-Pentadiyne, 1-(methylthio)-	110	C6H6S	042875-80-9	25
3			trans-1,4-Cyclohexanedimethanol,...	240	C10H15F3O3	1000385-95-3	17
4			2,3-Dimethyl-cyclohexa-1,3-diene	108	C8H12	004430-91-5	14
5			1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	12



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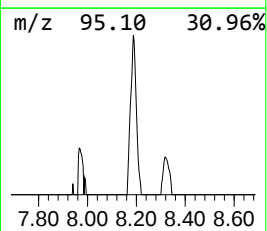
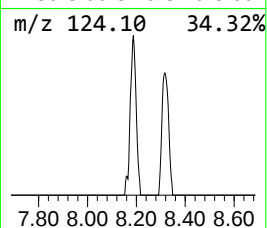
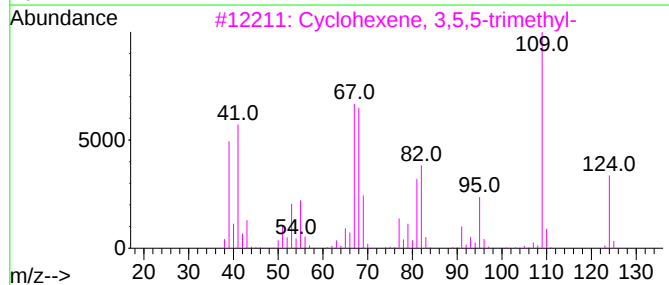
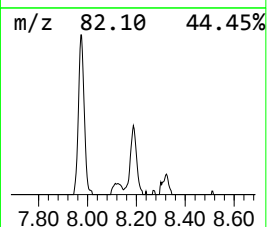
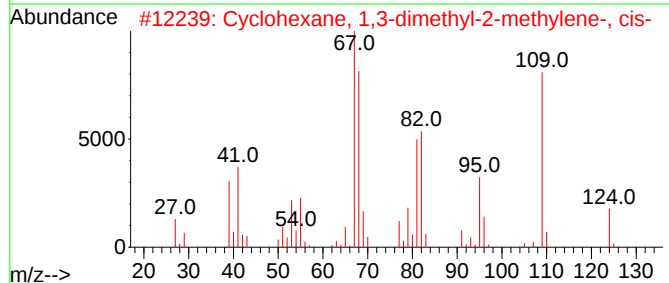
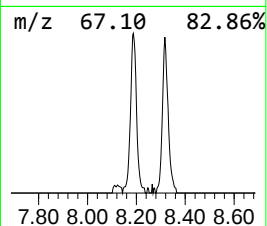
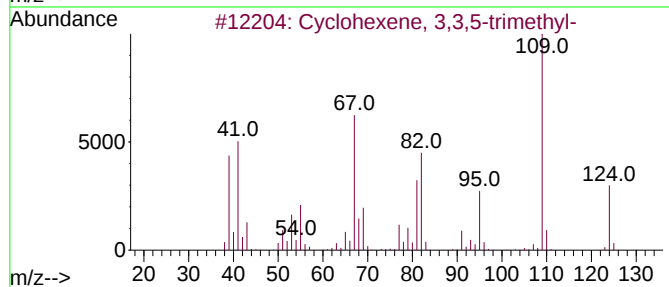
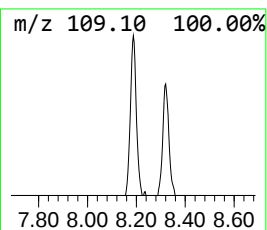
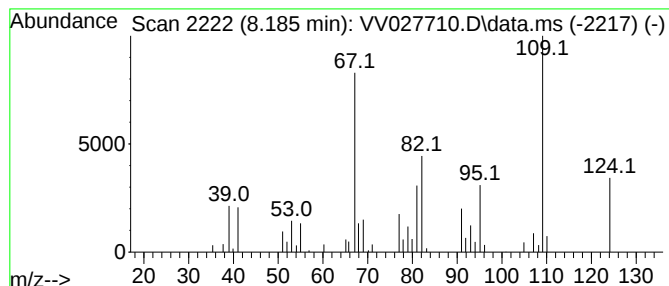
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Cyclohexene, 3,3,5-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.185	0.91 ug/L	62253	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	89
2			Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	019781-47-6	87
3			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	86
4			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	86
5			2,4-Heptadiene, 2,4-dimethyl-	124	C9H16	074421-05-9	76



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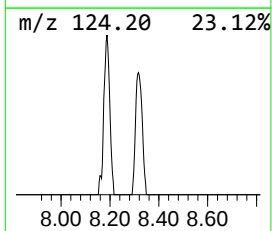
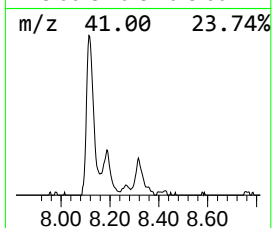
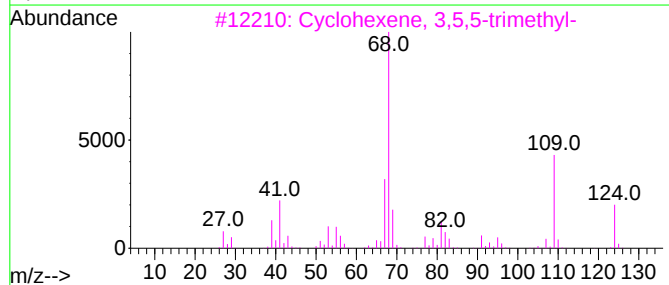
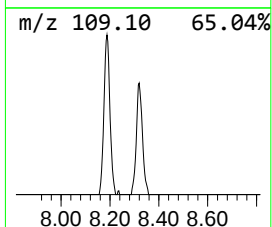
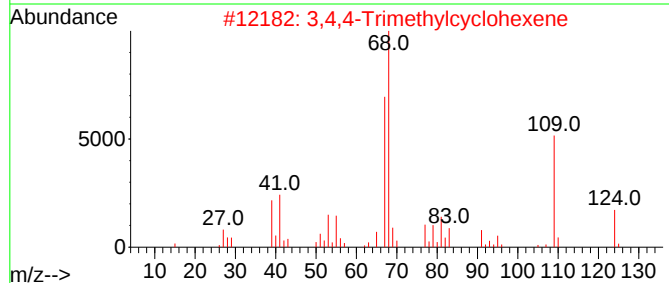
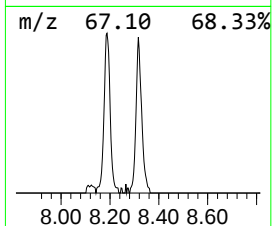
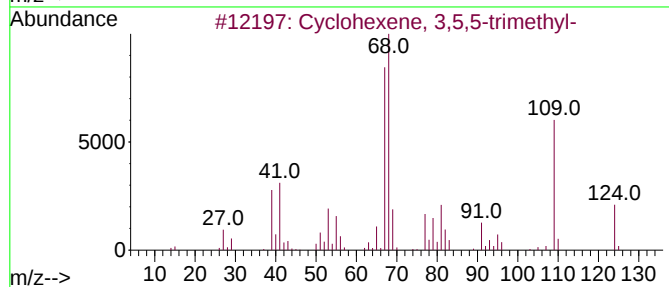
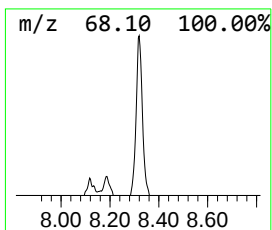
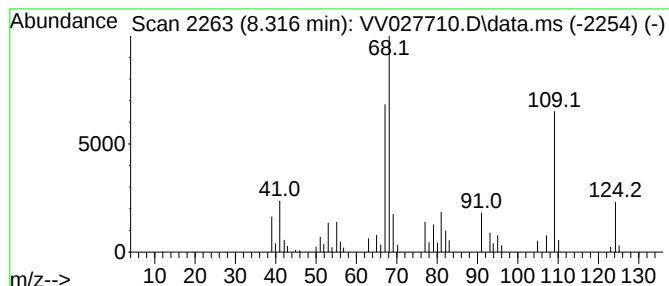
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexene, 3,5,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.316	0.85 ug/L	57856	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	95
2			3,4,4-Trimethylcyclohexene	124	C9H16	1000113-50-1	93
3			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	93
4			Cyclohexene, 1,6,6-trimethyl-	124	C9H16	069745-49-9	90
5			2,4-Heptadiene, 2,6-dimethyl-	124	C9H16	004634-87-1	60



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Quant Title : TRACE VOA SFAM1.0

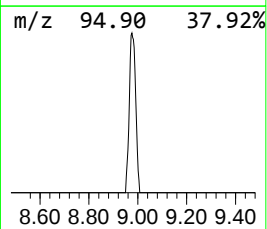
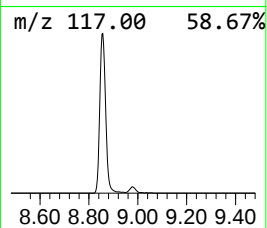
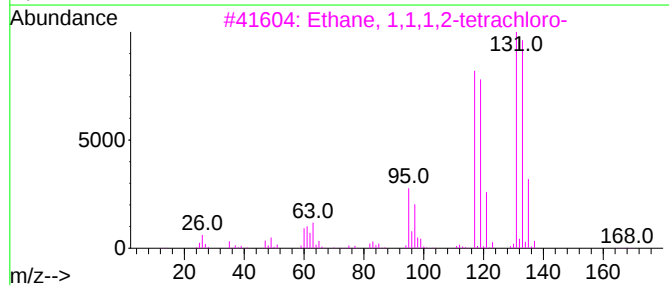
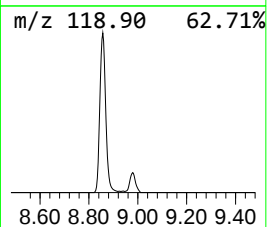
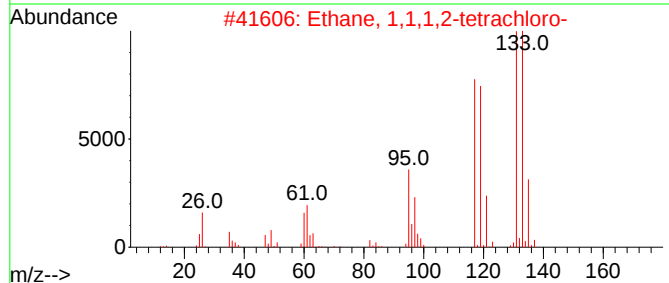
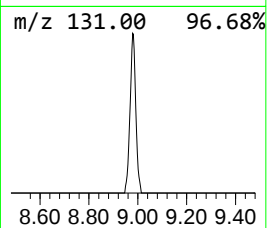
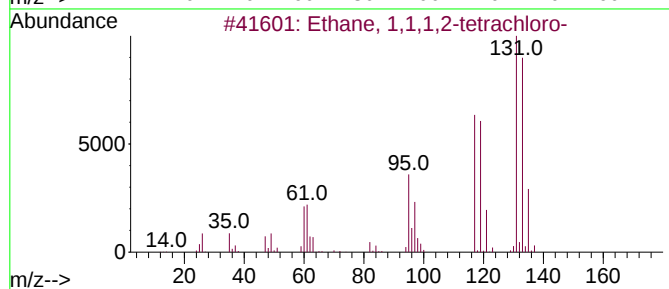
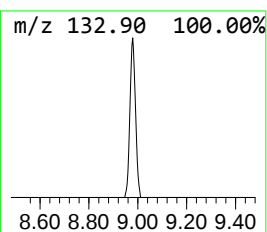
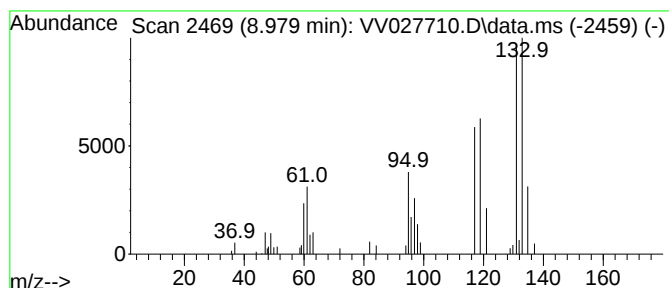
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.979	0.64 ug/L	43730	Chlorobenzene-d5	8.857

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	90
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	90
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	72
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	64
5			Carbon Tetrachloride	152	CCl4	000056-23-5	10



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Acq On : 02 Sep 2022 09:33
Operator : SY/MD
Sample : N4404-14
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 40 Sample Multiplier: 1

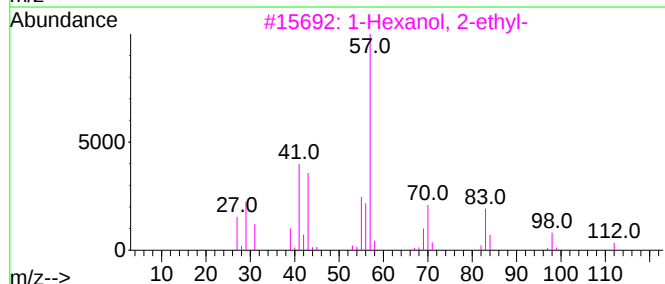
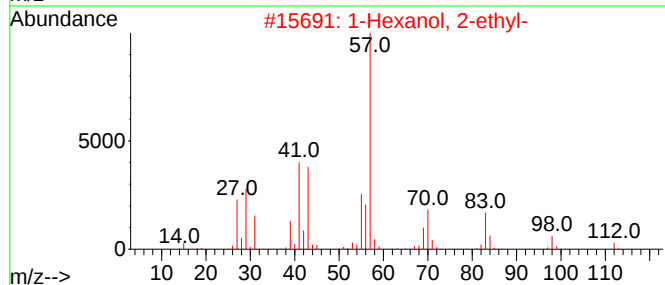
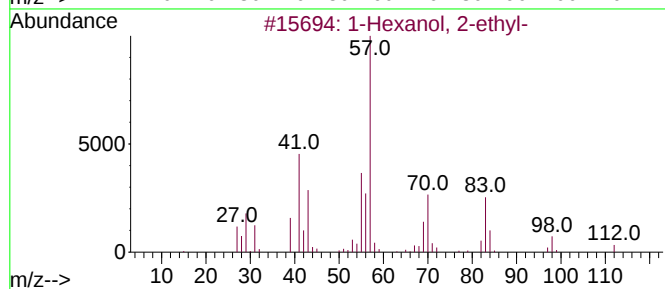
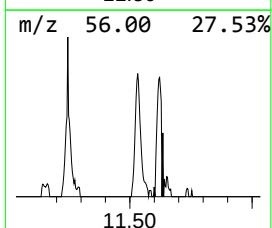
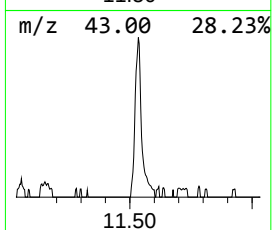
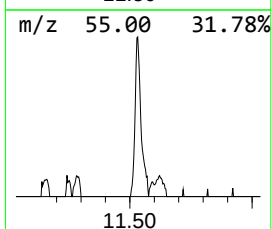
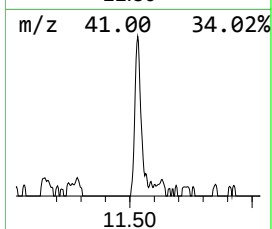
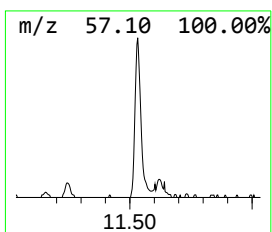
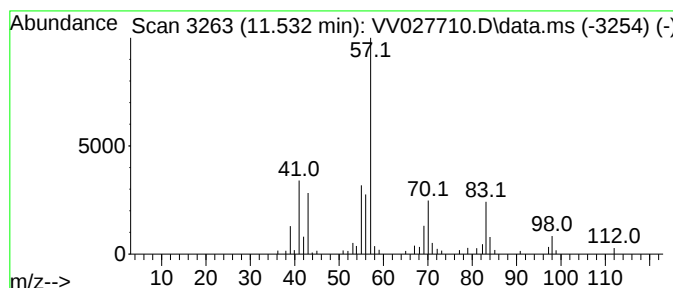
Instrument :
MSVOA_V
ClientSampleId :
DBVC5

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 7 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.532	0.80 ug/L	48623	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	90
2	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	74
4	1-Hexanol, 2-ethyl-		130	C8H18O	000104-76-7	72
5	1-Pentanol, 2-ethyl-4-methyl-		130	C8H18O	000106-67-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090122\
Data File : VV027710.D
Acq On : 02 Sep 2022 09:33
Operator : SY/MD
Sample : N4404-14
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBVC5

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
Sulfur dioxide	1.986	0.6	ug/L	38594	1	5.593	318390	5.0
Dimethyl selenide	3.108	1.0	ug/L	63355	1	5.593	318390	5.0
Cyclohexene, 3,...	8.185	0.9	ug/L	62253	2	8.857	342069	5.0
Cyclohexene, 3,...	8.316	0.8	ug/L	57856	2	8.857	342069	5.0
Ethane, 1,1,1,2...	8.979	0.6	ug/L	43730	2	8.857	342069	5.0
1-Hexanol, 2-et...	11.532	0.8	ug/L	48623	3	11.249	303509	5.0