

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090622\
 Data File : VV027752.D
 Acq On : 06 Sep 2022 19:40
 Operator : SY/MD
 Sample : N4404-14
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 17 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\SFAMVTR090622WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV027752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.298	73	80	91	rBV2	79093	88408	15.12%	1.622%
2	1.446	120	126	140	rVB6	10122	16068	2.75%	0.295%
3	1.564	156	163	172	rVB	66987	76925	13.16%	1.411%
4	2.111	323	333	349	rBV2	156947	227262	38.88%	4.169%
5	2.211	355	364	372	rBV2	16911	29335	5.02%	0.538%
6	2.294	386	390	396	rVB	6325	7682	1.31%	0.141%
7	3.111	634	644	659	rBV3	28269	56963	9.75%	1.045%
8	3.918	877	895	903	rBV2	57622	152380	26.07%	2.795%
9	4.365	1017	1034	1055	rBV4	109694	320215	54.78%	5.874%
10	5.040	1232	1244	1260	rBV2	281580	584516	100.00%	10.723%
11	5.600	1407	1418	1441	rVB	240067	507612	86.84%	9.312%
12	5.899	1498	1511	1532	rBV	59168	121964	20.87%	2.237%
13	6.072	1550	1565	1587	rBV	116894	248512	42.52%	4.559%
14	6.313	1629	1640	1652	rBV5	7210	13780	2.36%	0.253%
15	7.018	1846	1859	1881	rBV	50118	92277	15.79%	1.693%
16	7.339	1947	1959	1981	rBV	215009	374529	64.08%	6.871%
17	7.648	2045	2055	2071	rBV	30102	53577	9.17%	0.983%
18	7.866	2114	2123	2135	rVB6	8181	14366	2.46%	0.264%
19	7.992	2145	2162	2180	rBV	200956	343442	58.76%	6.300%
20	8.120	2191	2202	2219	rBV	202473	397652	68.03%	7.295%
21	8.201	2220	2227	2239	rVB3	32005	58523	10.01%	1.074%
22	8.333	2257	2268	2288	rVB4	25394	50670	8.67%	0.930%
23	8.863	2421	2433	2452	rBV	241620	399144	68.29%	7.322%
24	8.985	2461	2471	2484	rVB2	26619	43264	7.40%	0.794%
25	9.153	2513	2523	2538	rBV2	9081	14049	2.40%	0.258%
26	9.741	2694	2706	2715	rBV2	13880	22859	3.91%	0.419%
27	10.220	2843	2855	2869	rBV2	83078	132745	22.71%	2.435%
28	11.249	3164	3175	3197	rBV	230343	359881	61.57%	6.602%
29	11.532	3251	3263	3277	rBV	48236	83650	14.31%	1.535%
30	11.625	3281	3292	3311	rVB	205379	325077	55.61%	5.963%
31	12.345	3507	3516	3525	rVB7	8206	11670	2.00%	0.214%
32	15.898	4595	4621	4656	rBV7	36129	222123	38.00%	4.075%

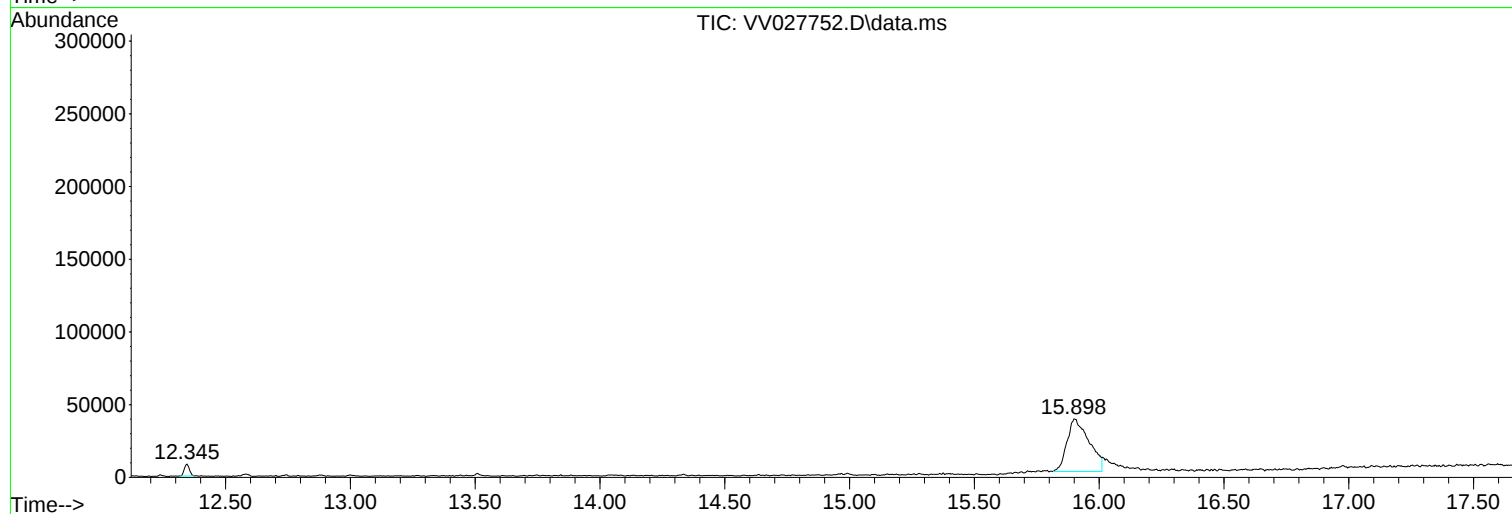
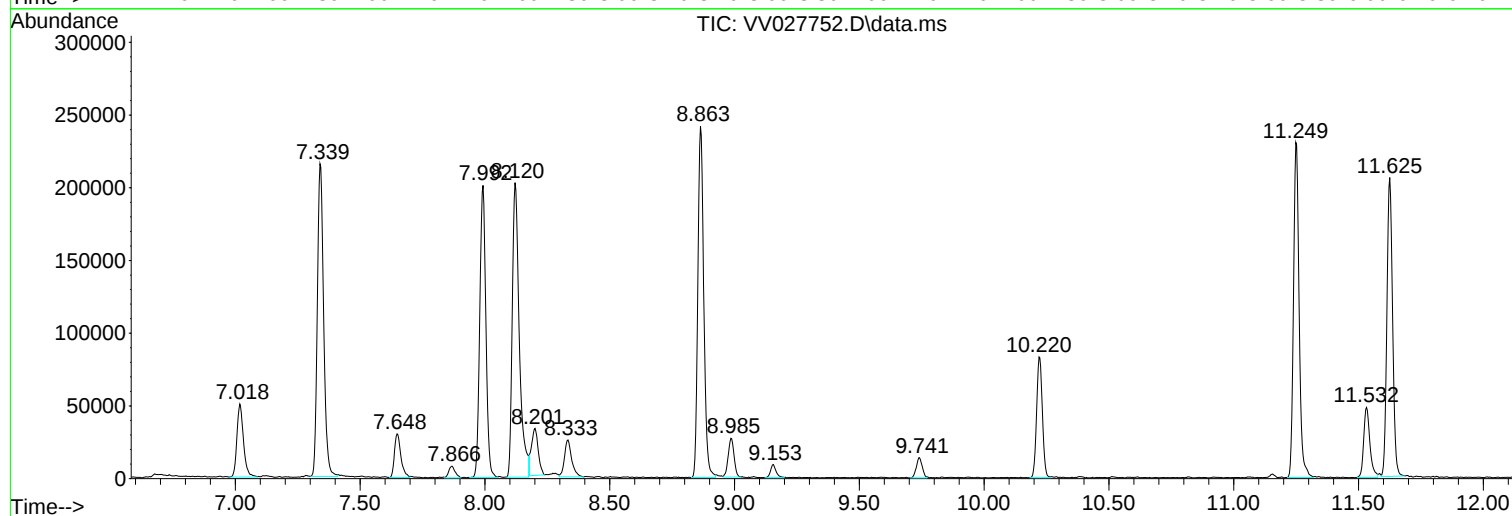
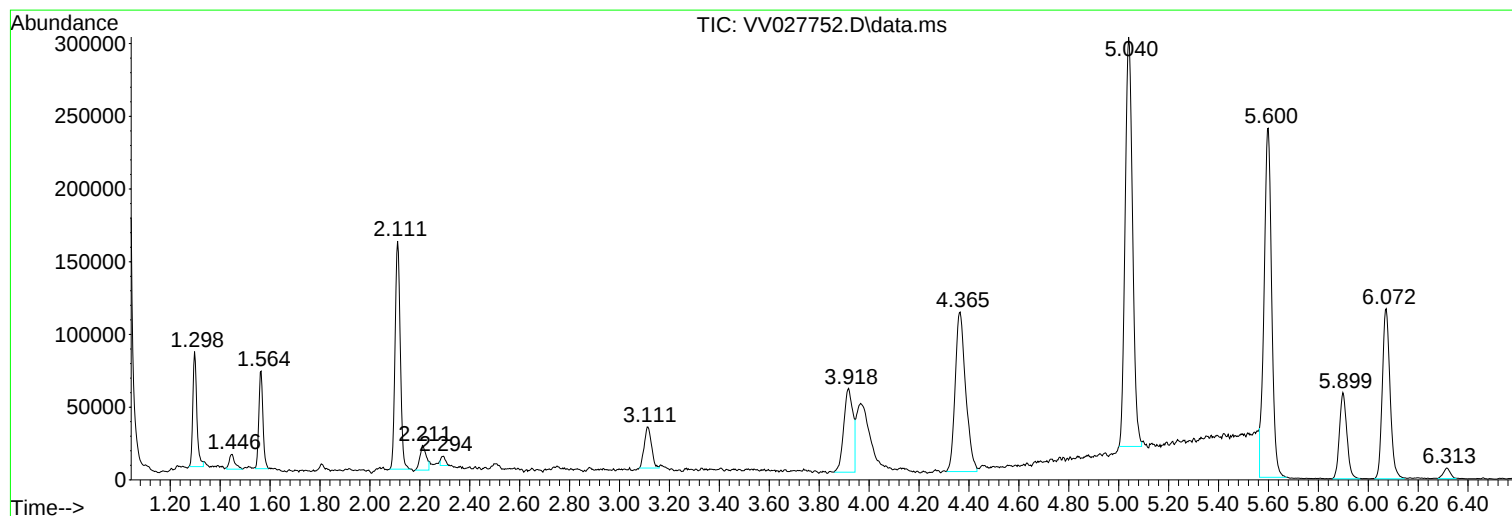
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR090622WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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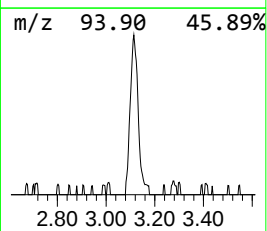
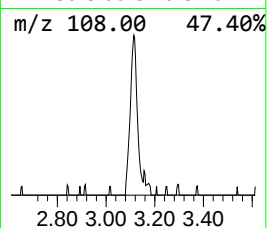
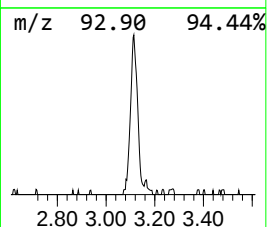
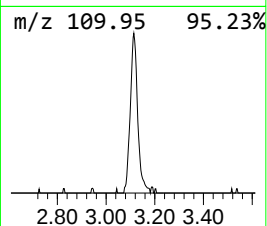
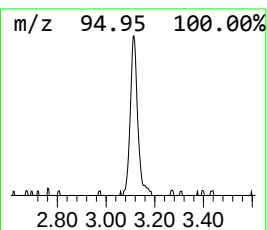
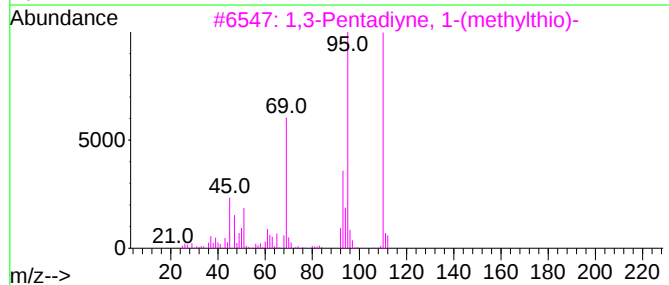
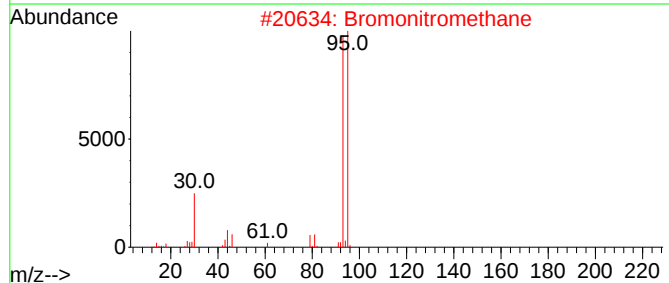
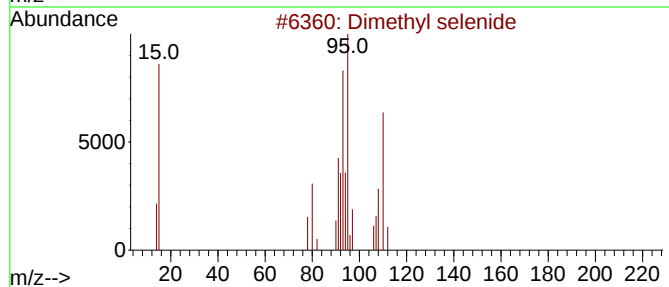
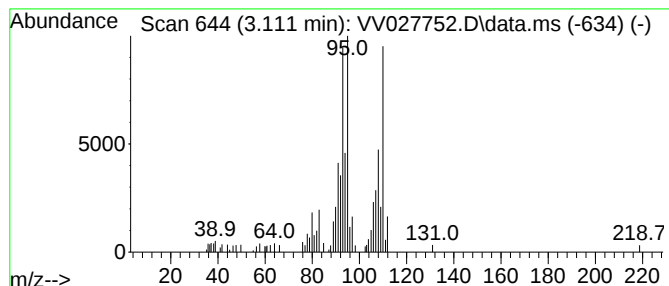
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR090622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Dimethyl selenide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.111	0.56 ug/L	56963	1,4-Difluorobenzene	5.600

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl selenide	110	C2H6Se	000593-79-3	81
2			Bromonitromethane	139	CH2BrNO2	000563-70-2	27
3			1,3-Pentadiyne, 1-(methylthio)-	110	C6H6S	042875-80-9	25
4			1H-Imidazole,1-ethyl-2-methyl	110	C6H10N2	021202-52-8	22
5			1H-Imidazole, 2-ethyl-4-methyl-	110	C6H10N2	000931-36-2	16



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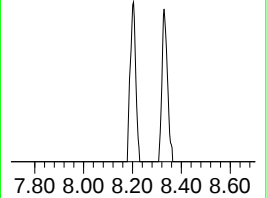
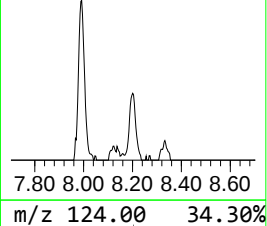
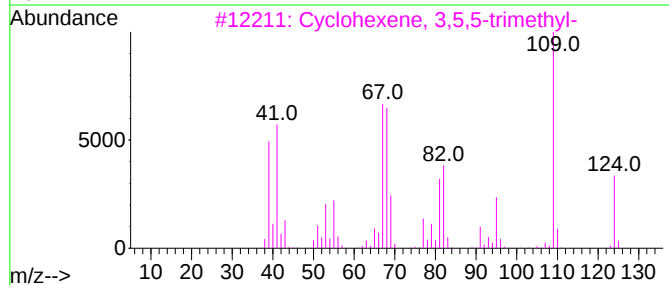
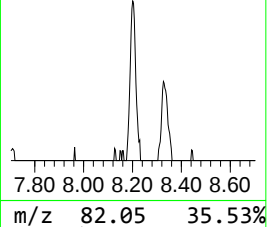
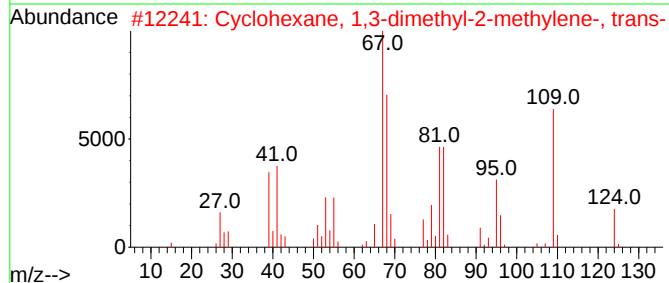
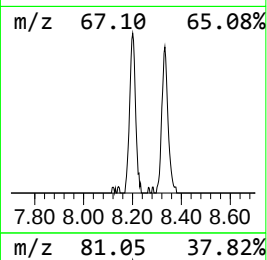
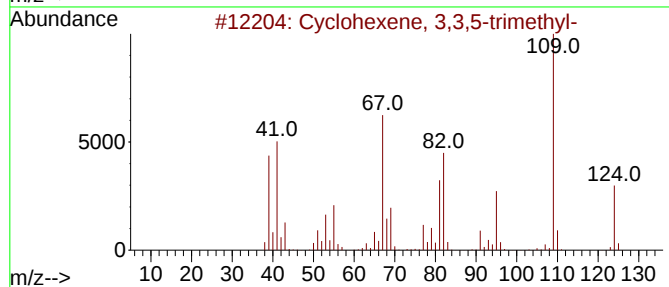
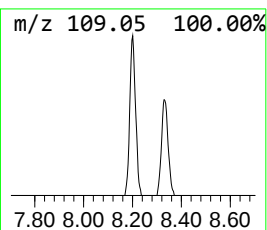
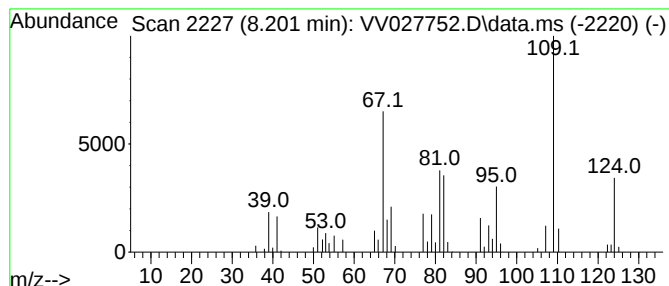
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR090622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.201	0.73 ug/L	58523	Chlorobenzene-d5	8.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	93
2			Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	020348-74-7	87
3			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	83
4			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	78
5			1,3-Heptadiene, 2,3-dimethyl-	124	C9H16	074779-65-0	64



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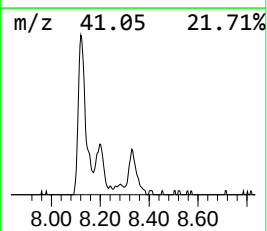
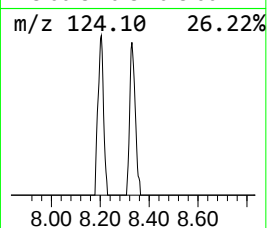
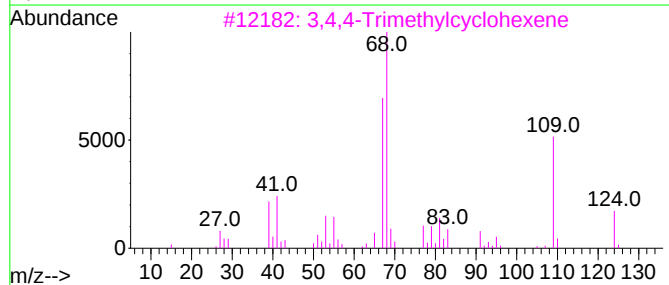
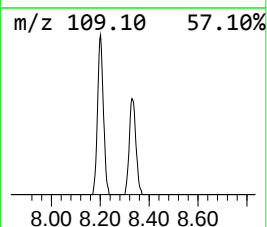
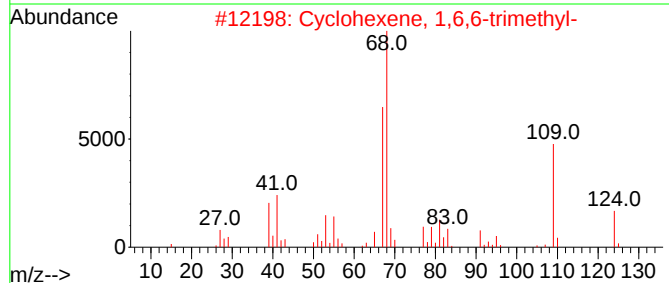
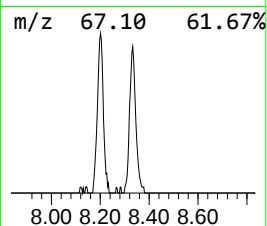
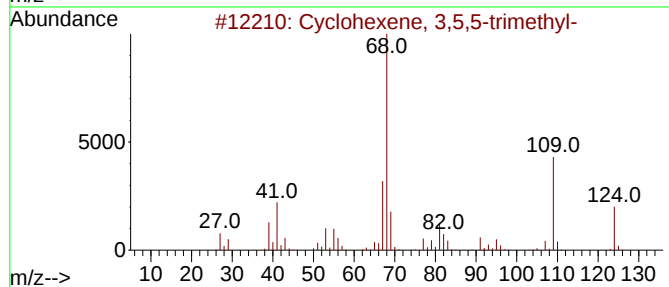
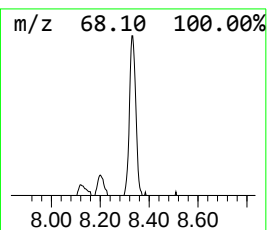
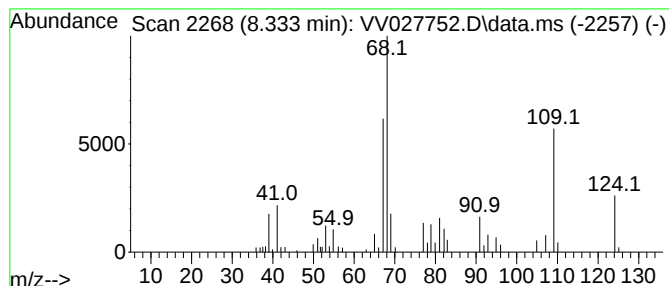
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR090622WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.333	0.63 ug/L	50670	Chlorobenzene-d5	8.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	94
2			Cyclohexene, 1,6,6-trimethyl-	124	C9H16	069745-49-9	90
3			3,4,4-Trimethylcyclohexene	124	C9H16	1000113-50-1	87
4			Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	64
5			Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	49



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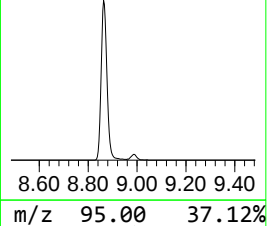
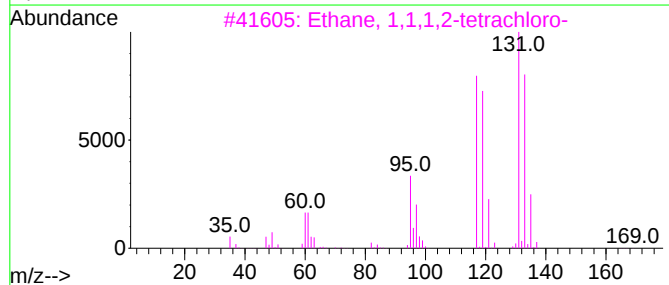
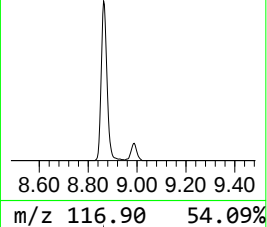
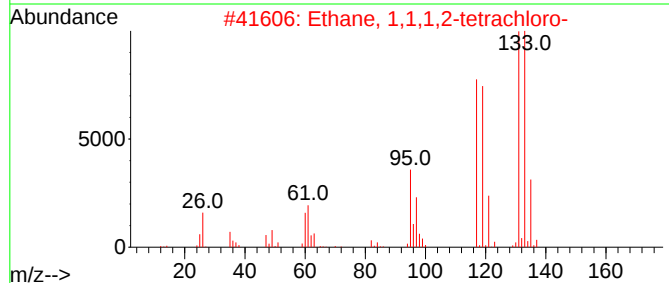
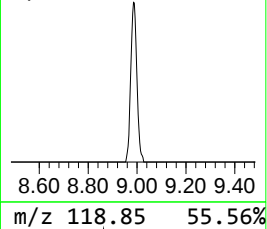
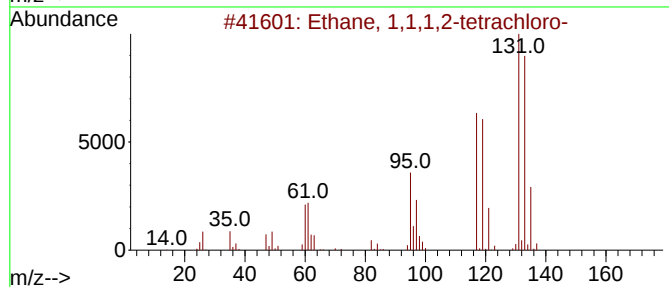
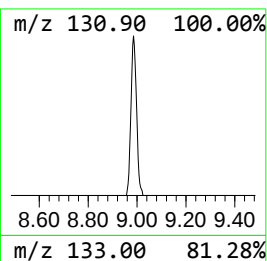
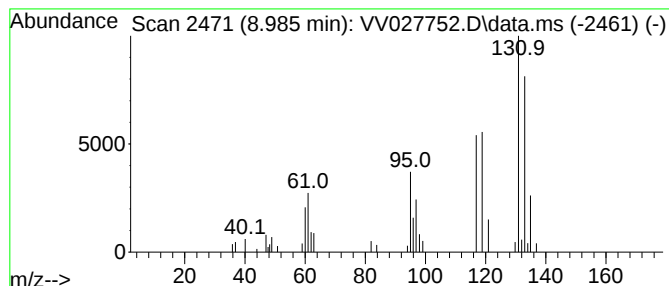
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.985	0.54 ug/L	43264	Chlorobenzene-d5	8.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	83
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	72
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	59
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	56
5			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	9



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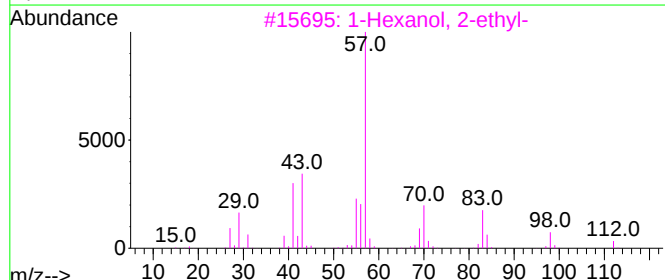
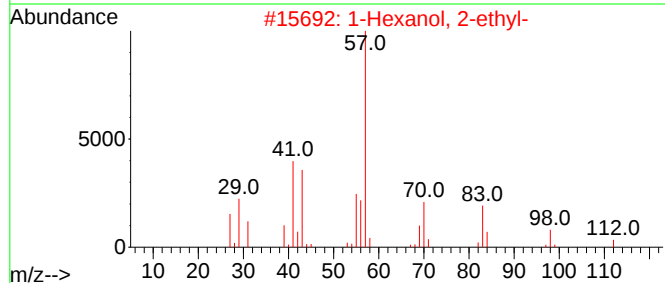
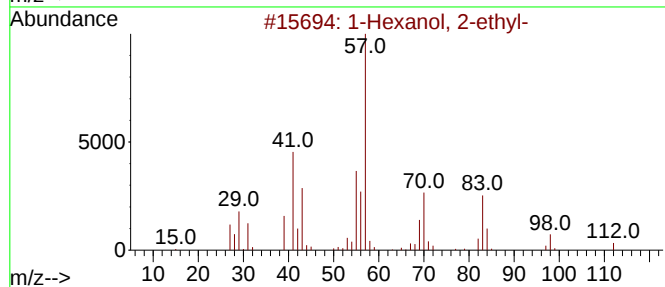
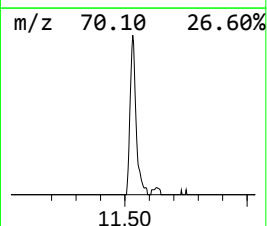
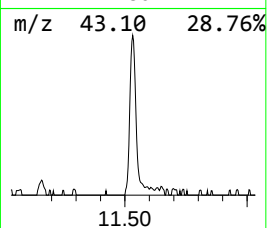
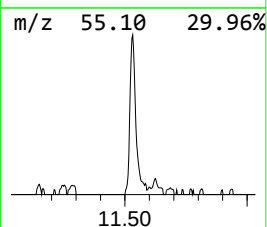
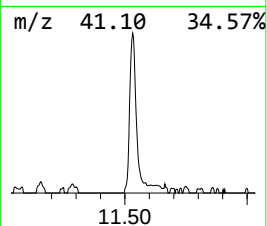
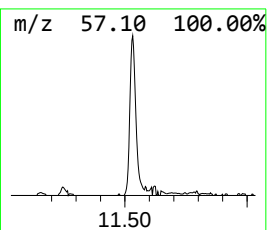
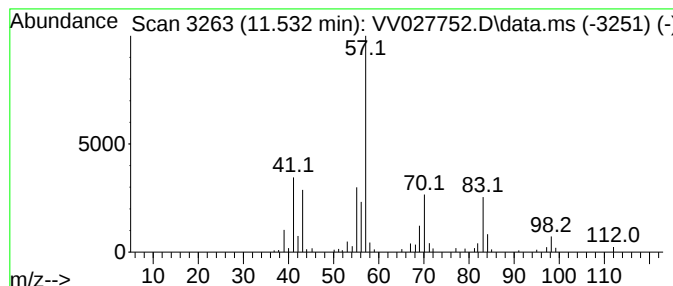
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.532	1.16 ug/L	83650	1,4-Dichlorobenzene-d4	11.252

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	83
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64



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ClientSampleId :
DBVC5

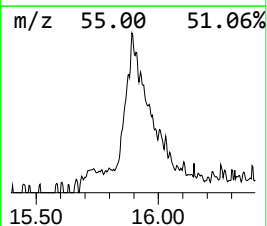
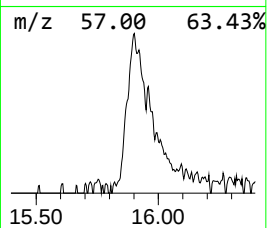
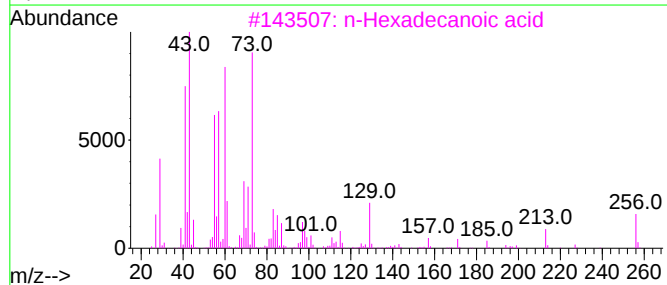
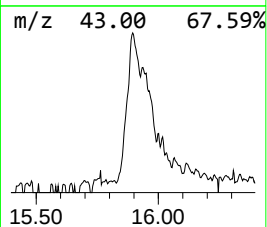
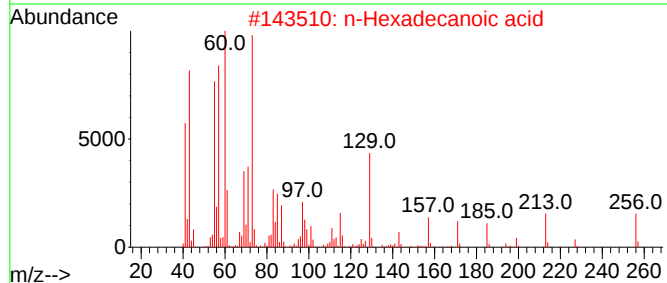
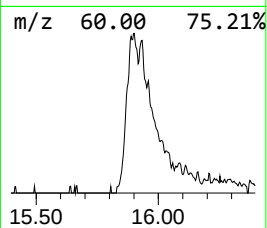
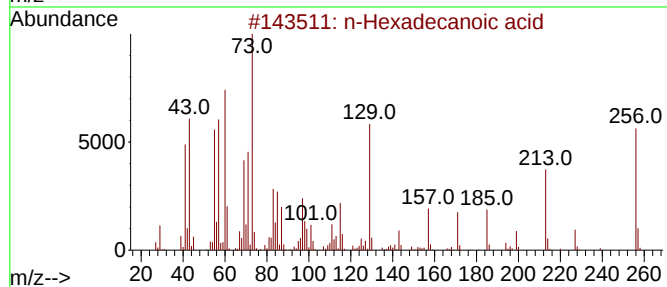
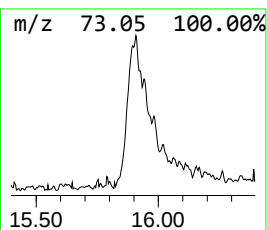
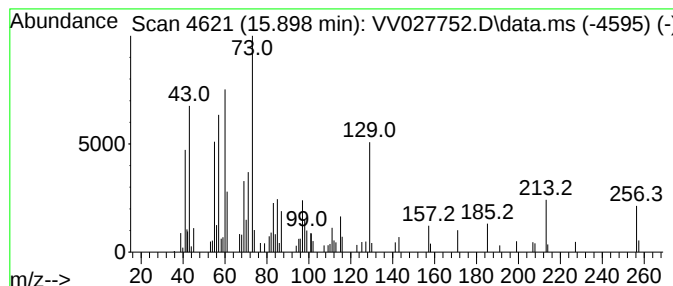
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	3.09 ug/L	222123	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV090622\
Data File : VV027752.D
Acq On : 06 Sep 2022 19:40
Operator : SY/MD
Sample : N4404-14
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBVC5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR090622WMA.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
Dimethyl selenide	3.111	0.6	ug/L	56963	1	5.600	507612	5.0
Cyclohexene, 3,...	8.201	0.7	ug/L	58523	2	8.863	399144	5.0
Cyclohexene, 3,...	8.333	0.6	ug/L	50670	2	8.863	399144	5.0
Ethane, 1,1,1,2...	8.985	0.5	ug/L	43264	2	8.863	399144	5.0
1-Hexanol, 2-et...	11.532	1.2	ug/L	83650	3	11.252	359881	5.0
n-Hexadecanoic ...	15.898	3.1	ug/L	222123	3	11.252	359881	5.0