

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121523\
 Data File : VU056879.D
 Acq On : 15 Dec 2023 15:10
 Operator : MD/SY
 Sample : 05677-11
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H0AC7

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_U\Method\SFAMUTR121123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU056879.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.515	64	70	80	rBV2	10471	12090	1.21%	0.137%
2	1.596	80	95	110	rVB	135952	173455	17.38%	1.962%
3	1.911	184	193	209	rBV	109628	150790	15.11%	1.706%
4	2.448	351	360	372	rVB2	56464	95281	9.55%	1.078%
5	2.563	383	396	413	rBV	221139	365600	36.64%	4.136%
6	3.039	533	544	558	rBV2	7380	13267	1.33%	0.150%
7	4.637	1027	1041	1088	rBV2	87417	364496	36.53%	4.124%
8	5.055	1153	1171	1194	rBV	201847	453868	45.49%	5.135%
9	5.721	1358	1378	1407	rBV2	383833	997765	100.00%	11.288%
10	6.245	1525	1541	1572	rBV	264839	527816	52.90%	5.971%
11	6.685	1664	1678	1700	rBV	237830	471881	47.29%	5.338%
12	7.563	1936	1951	1974	rBV	107300	203873	20.43%	2.306%
13	7.894	2041	2054	2072	rBV	427943	773568	77.53%	8.751%
14	7.968	2072	2077	2094	rVB2	10222	19312	1.94%	0.218%
15	8.177	2131	2142	2168	rBV3	66180	120150	12.04%	1.359%
16	8.470	2225	2233	2249	rVV5	10091	19780	1.98%	0.224%
17	8.547	2249	2257	2267	rVB7	6568	11932	1.20%	0.135%
18	8.631	2272	2283	2317	rBV2	450769	948651	95.08%	10.732%
19	9.415	2513	2527	2550	rBV	380406	676153	67.77%	7.649%
20	10.750	2931	2942	2959	rBV	171016	274630	27.52%	3.107%
21	10.885	2973	2984	2998	rVB2	14434	24117	2.42%	0.273%
22	11.807	3259	3271	3294	rBV	352938	593550	59.49%	6.715%
23	12.061	3341	3350	3367	rBV3	16109	27772	2.78%	0.314%
24	12.187	3377	3389	3416	rBV	387551	678884	68.04%	7.680%
25	14.309	4039	4049	4063	rBV2	99062	157021	15.74%	1.776%
26	15.685	4464	4477	4487	rBV3	59425	98195	9.84%	1.111%
27	16.762	4801	4812	4837	rBV2	338503	585461	58.68%	6.623%

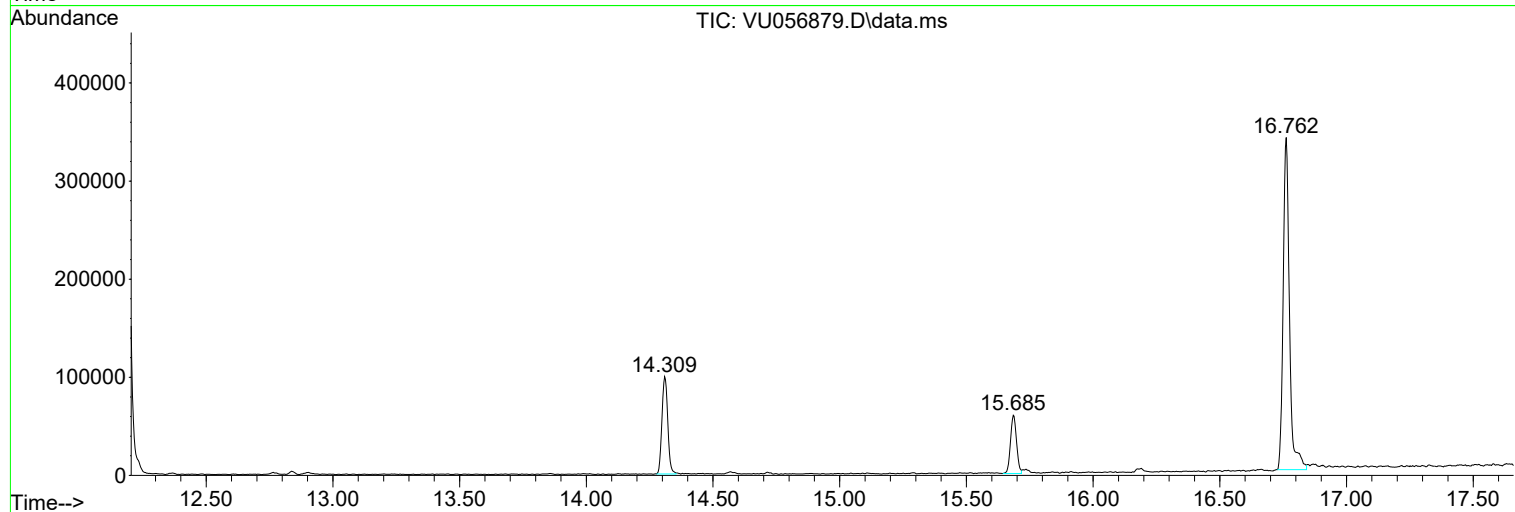
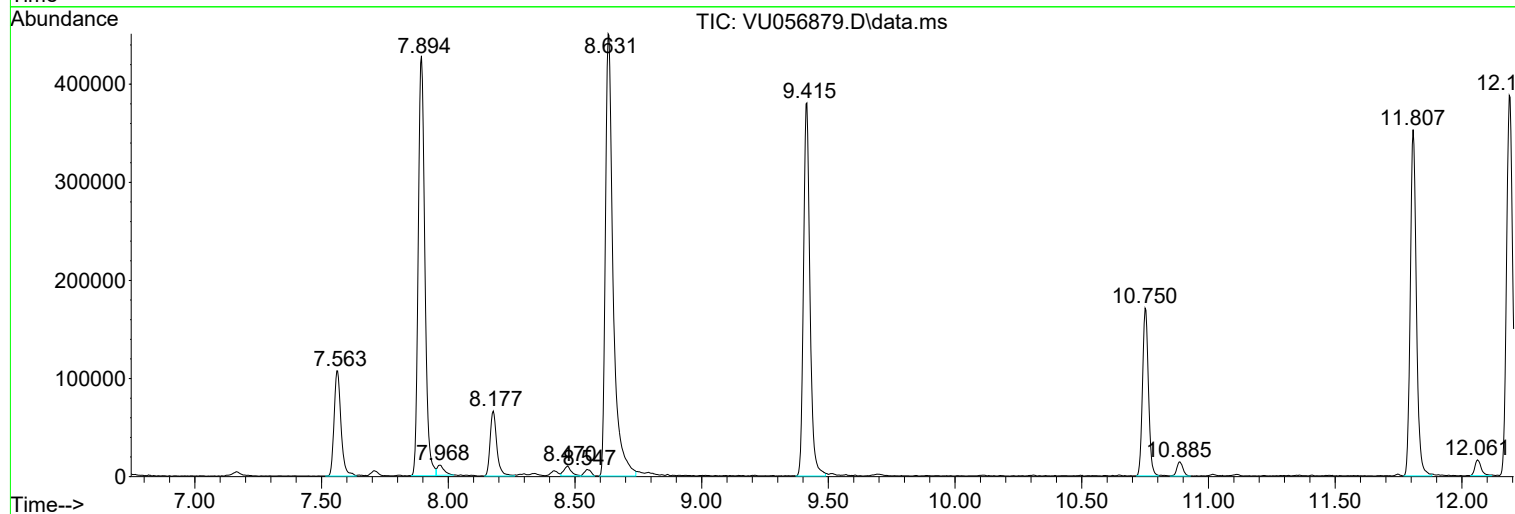
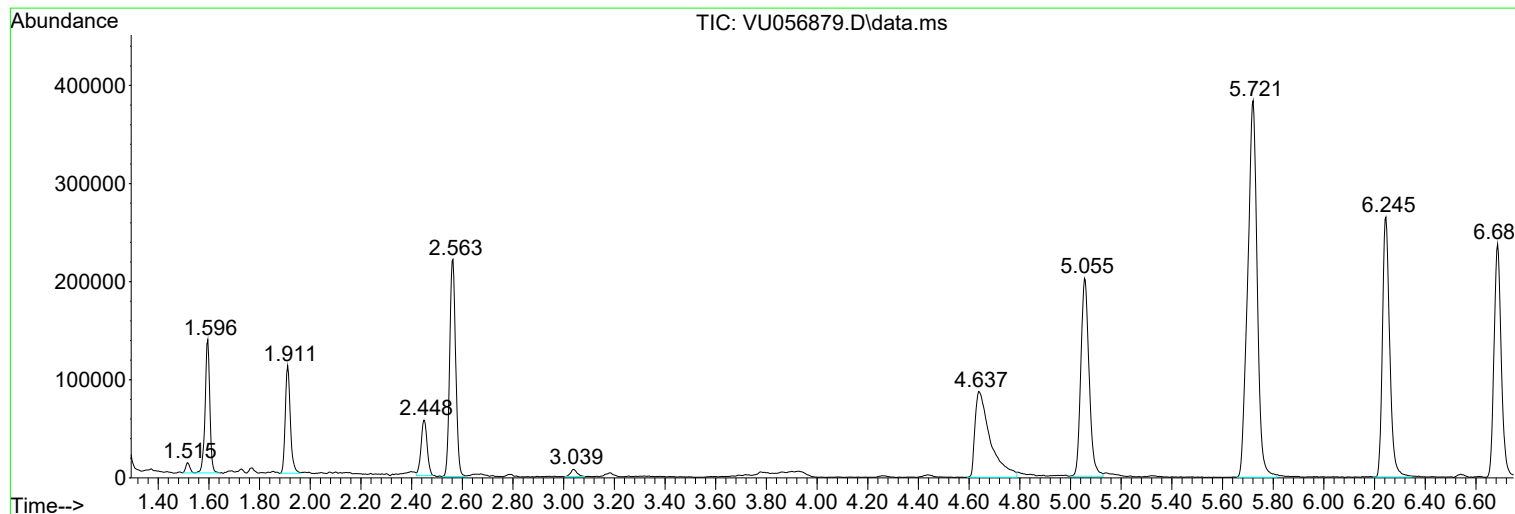
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H0AC7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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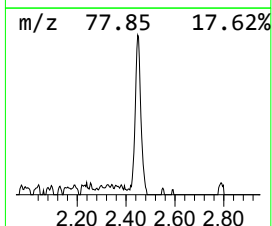
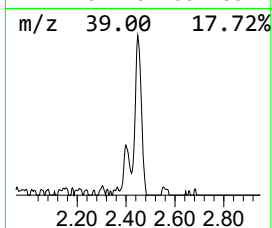
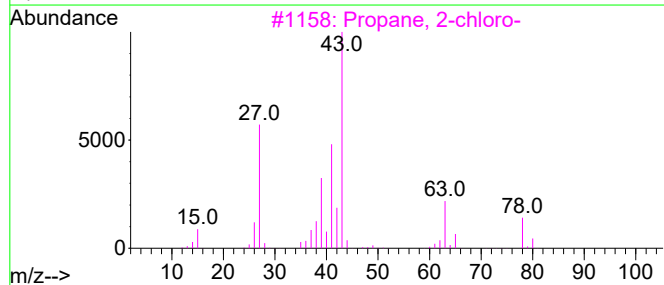
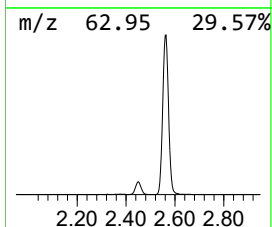
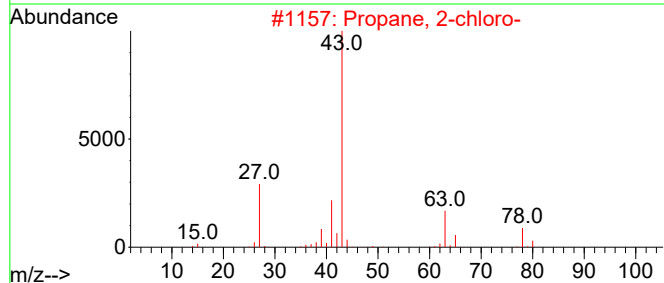
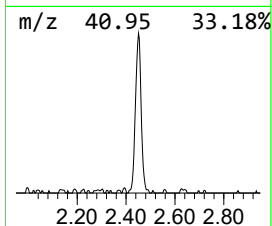
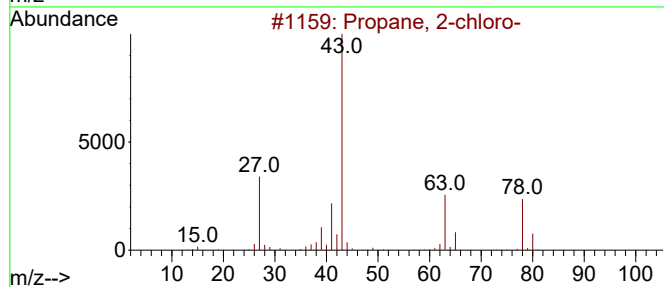
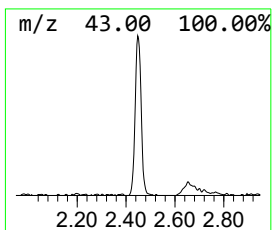
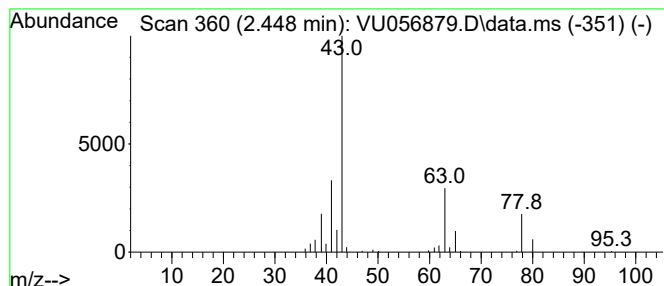
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Propane, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.448	0.90 ug/L	95281	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-chloro-			78	C3H7Cl	000075-29-6	74
2	Propane, 2-chloro-			78	C3H7Cl	000075-29-6	64
3	Propane, 2-chloro-			78	C3H7Cl	000075-29-6	59
4	2-Chloroethanol			80	C2H5ClO	000107-07-3	5
5	Ethene, (methylsulfonyl)-			106	C3H6O2S	003680-02-2	4



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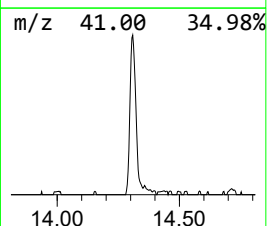
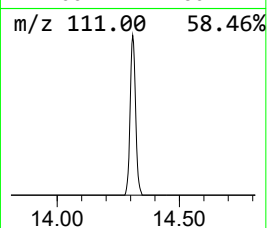
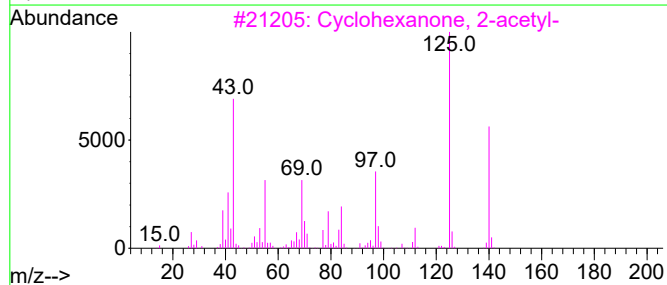
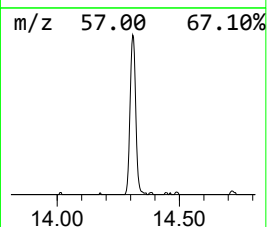
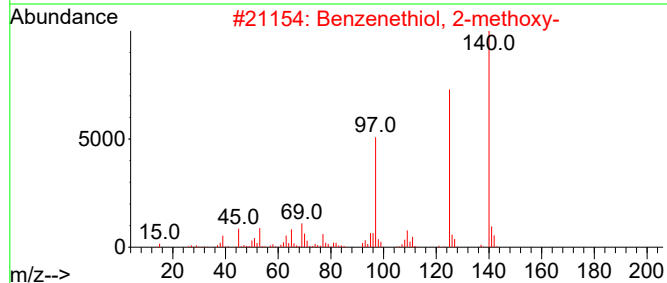
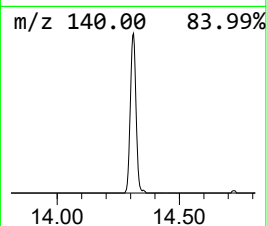
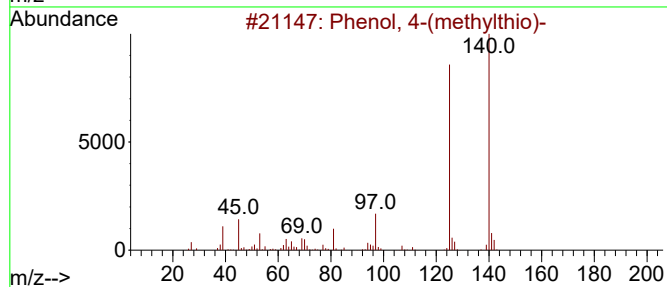
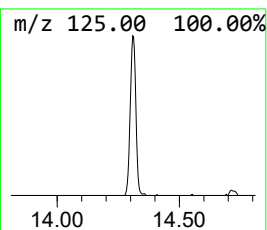
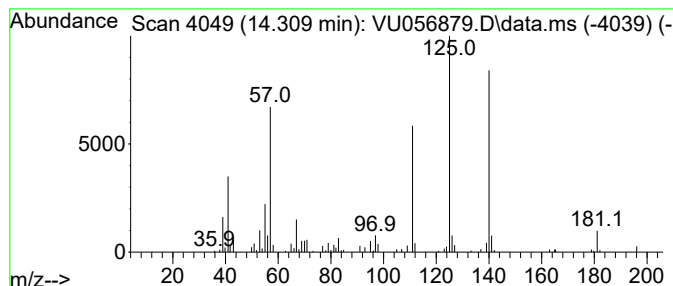
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Phenol, 4-(methylthio)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.309	1.32 ug/L	157021	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	59
2			Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	59
3			Cyclohexanone, 2-acetyl-	140	C8H12O2	000874-23-7	59
4			Artedouglasia oxide A	250	C15H22O3	115403-96-8	59
5			1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59



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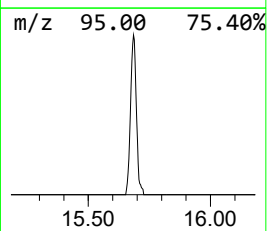
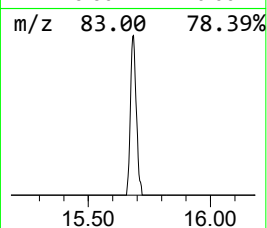
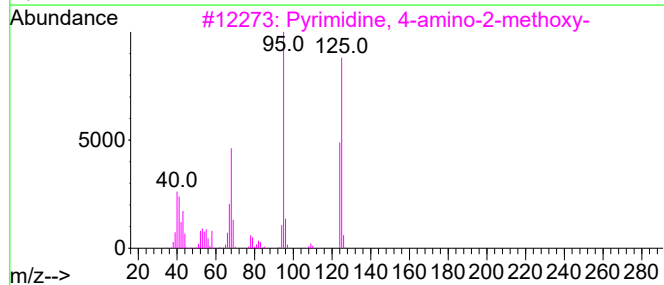
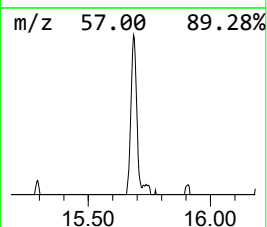
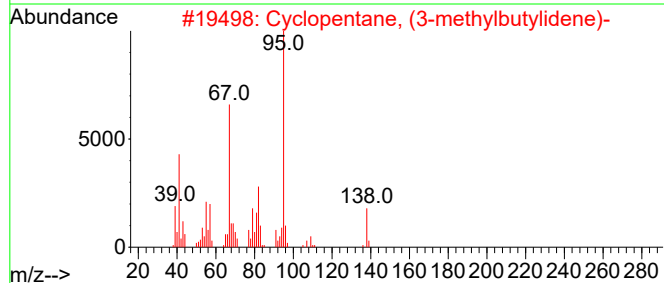
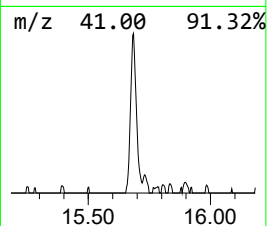
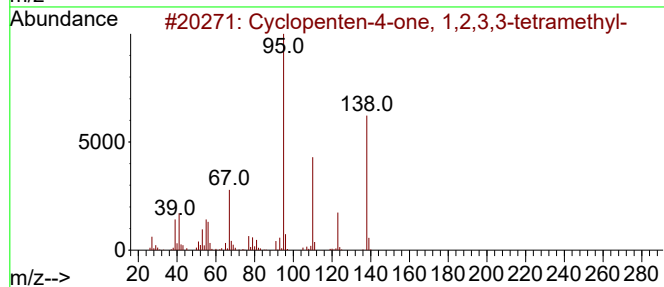
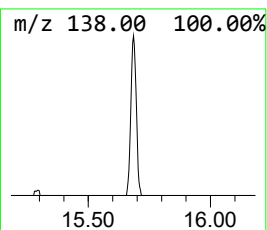
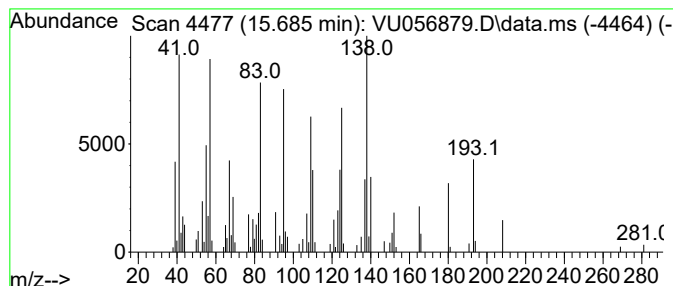
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.685	0.83 ug/L	98195	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopenten-4-one, 1,2,3,3-tetra...	138	C9H14O	1000163-38-6	30
2			Cyclopentane, (3-methylbutylidene)-	138	C10H18	053366-51-1	30
3			Pyrimidine, 4-amino-2-methoxy-	125	C5H7N3O	003289-47-2	25
4			1,2-Dimethyl-4-oxocyclohex-2-ene...	152	C9H12O2	1000187-01-2	20
5			Pyrazine, 2-methoxy-3-(1-methylp...	166	C9H14N2O	024168-70-5	18



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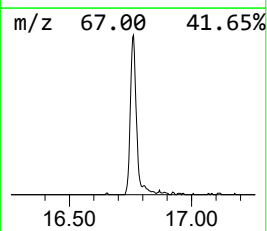
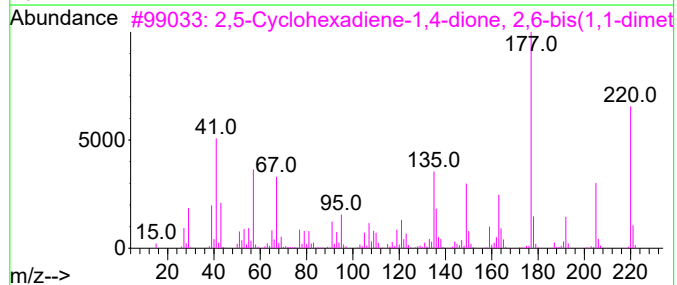
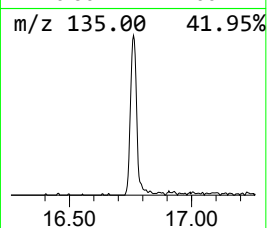
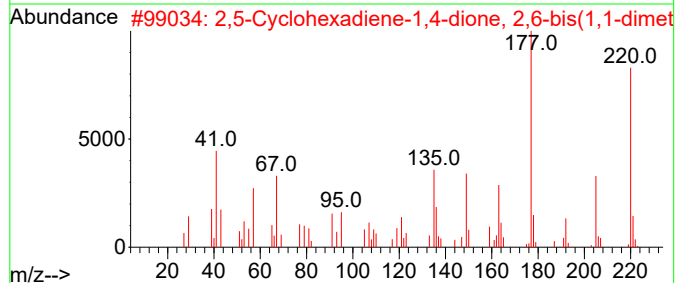
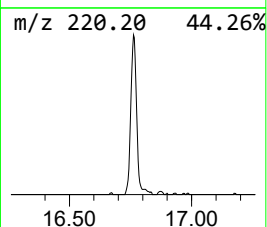
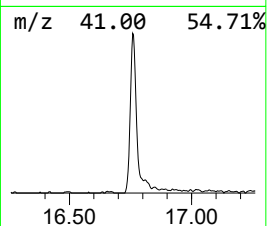
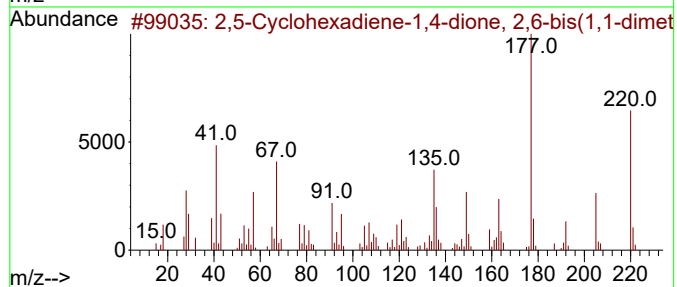
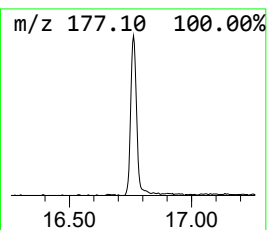
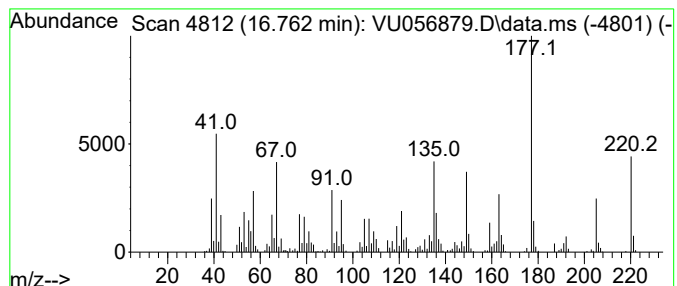
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Peak Number 5 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	4.93 ug/L	585461	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	95		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	91		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	91		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	83		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2-chloro-	2.448	0.9	ug/L	95281	1	6.245	527816	5.0
Phenol, 4-(meth...	14.309	1.3	ug/L	157021	3	11.807	593550	5.0
unknown-01	15.685	0.8	ug/L	98195	3	11.807	593550	5.0
2,5-Cyclohexadi...	16.762	4.9	ug/L	585461	3	11.807	593550	5.0