

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082923\
 Data File : VU054956.D
 Acq On : 29 Aug 2023 14:55
 Operator : MD/SY
 Sample : 04158-09
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AR1

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\SFAMUTR082823WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU054956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.518	65	71	79	rBV2	7707	10610	1.40%	0.187%
2	1.596	89	95	108	rVB	35209	41268	5.46%	0.728%
3	1.686	116	123	134	rVB	17284	21420	2.84%	0.378%
4	1.908	185	192	206	rVB	46465	60706	8.04%	1.071%
5	2.563	385	396	409	rBV	74254	120289	15.93%	2.121%
6	2.637	409	419	437	rVV	13361	27256	3.61%	0.481%
7	3.043	535	545	555	rVB4	4739	9230	1.22%	0.163%
8	3.187	576	590	602	rBV2	4328	9535	1.26%	0.168%
9	4.628	1026	1038	1069	rBV2	114996	321785	42.60%	5.675%
10	5.059	1158	1172	1194	rBV	106649	240287	31.81%	4.238%
11	5.724	1359	1379	1403	rBV2	198928	527367	69.82%	9.301%
12	6.248	1529	1542	1561	rBV	222475	436852	57.84%	7.704%
13	6.689	1664	1679	1696	rBV	138092	276443	36.60%	4.875%
14	7.566	1940	1952	1966	rBV3	55897	105064	13.91%	1.853%
15	7.798	2014	2024	2037	rBV5	5162	10112	1.34%	0.178%
16	7.898	2042	2055	2069	rBV	238140	416937	55.20%	7.353%
17	7.968	2069	2077	2094	rVB	28051	52366	6.93%	0.924%
18	8.181	2131	2143	2160	rBV2	33439	60466	8.01%	1.066%
19	8.634	2269	2284	2316	rBV2	348676	755319	100.00%	13.321%
20	9.415	2514	2527	2546	rBV	316745	545737	72.25%	9.625%
21	9.955	2682	2695	2707	rBV3	7973	15149	2.01%	0.267%
22	10.119	2732	2746	2754	rBV5	7665	16856	2.23%	0.297%
23	10.756	2931	2944	2959	rBV	123572	198429	26.27%	3.500%
24	10.894	2974	2987	2997	rBV3	5622	9399	1.24%	0.166%
25	11.479	3157	3169	3184	rBV7	8586	18245	2.42%	0.322%
26	11.811	3260	3272	3288	rBV	357188	571181	75.62%	10.074%
27	12.061	3341	3350	3364	rBV3	12502	24578	3.25%	0.433%
28	12.193	3378	3391	3410	rVB	279362	466089	61.71%	8.220%
29	12.566	3496	3507	3525	rBV2	50845	83916	11.11%	1.480%
30	13.213	3697	3708	3724	rBV4	10755	19461	2.58%	0.343%
31	13.676	3841	3852	3864	rBV8	5940	14520	1.92%	0.256%
32	14.074	3967	3976	3989	rBV8	4016	10487	1.39%	0.185%
33	14.209	4008	4018	4029	rBV3	44576	65831	8.72%	1.161%
34	14.341	4050	4059	4069	rVB4	13392	19951	2.64%	0.352%
35	14.573	4120	4131	4146	rVB2	4833	8381	1.11%	0.148%
36	14.740	4174	4183	4195	rVB	52275	78582	10.40%	1.386%

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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\SFAMUTR082823WMA.M
Title : TRACE VOA SFAM1.0

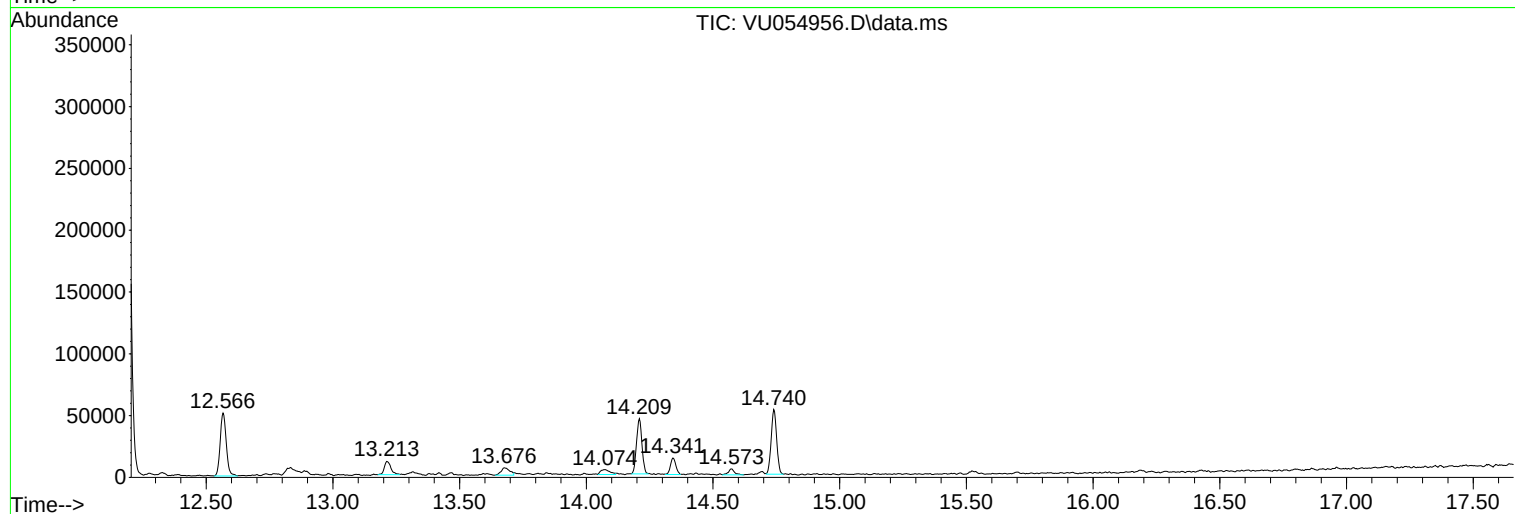
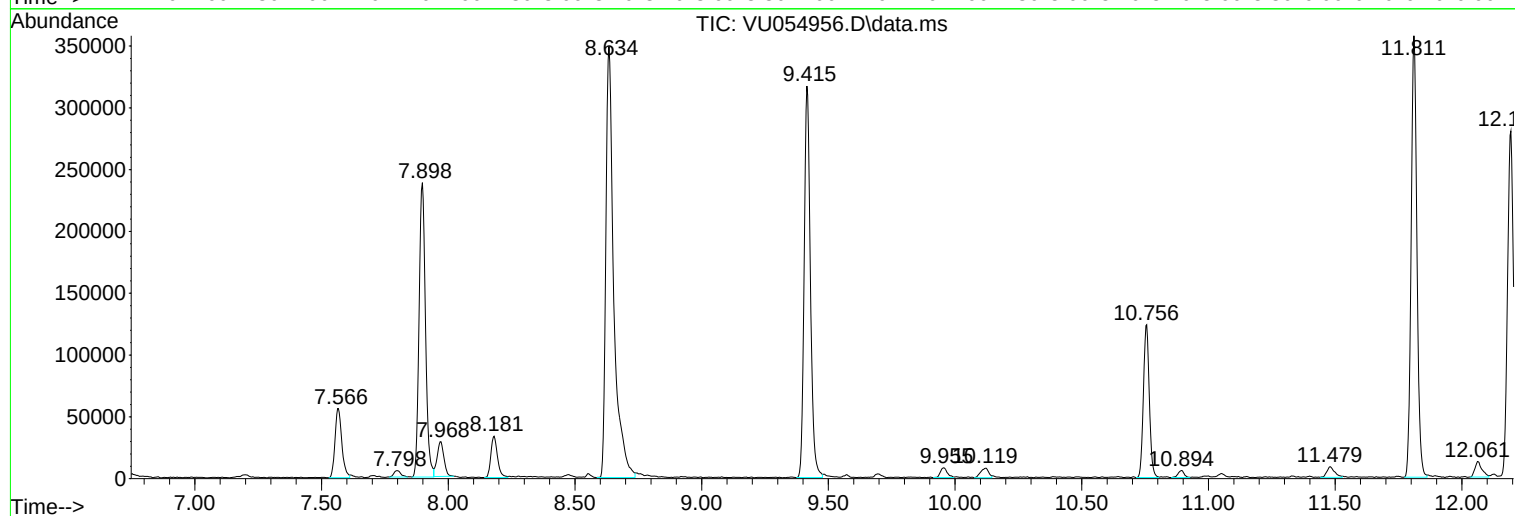
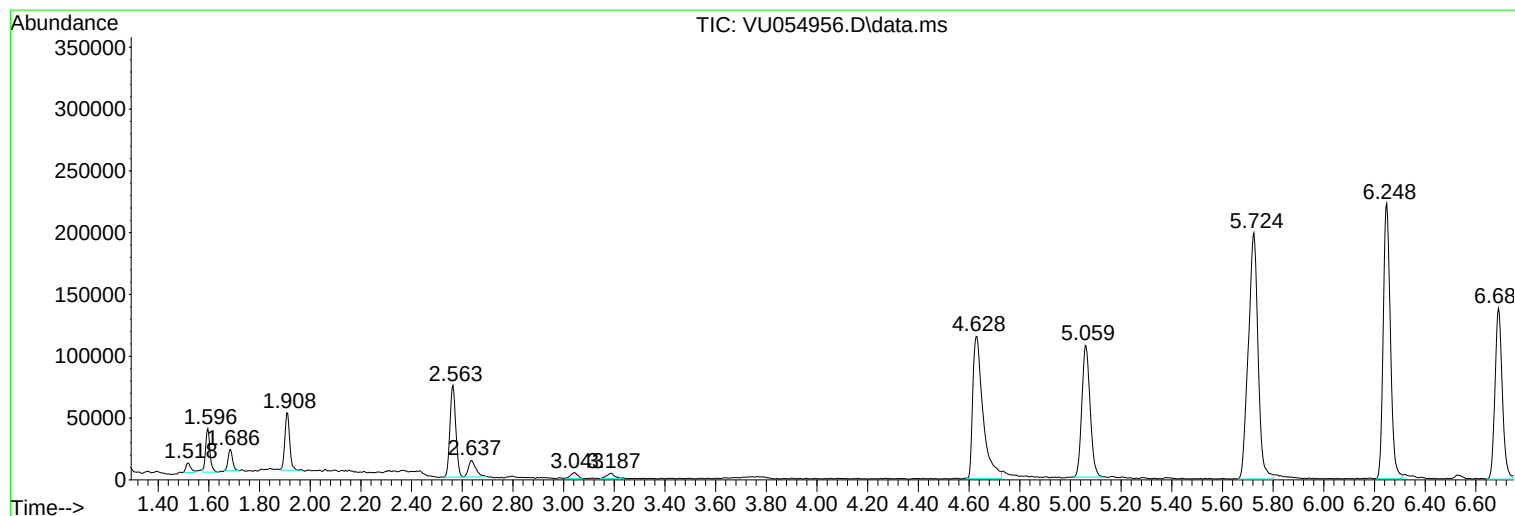
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR082823WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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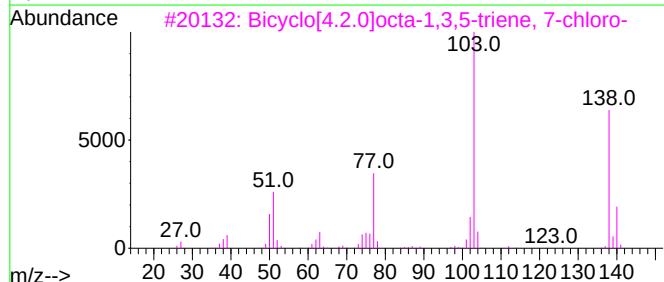
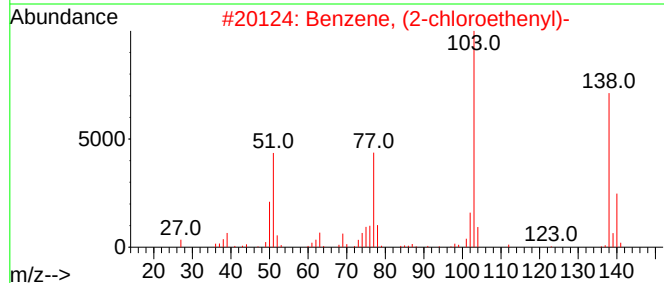
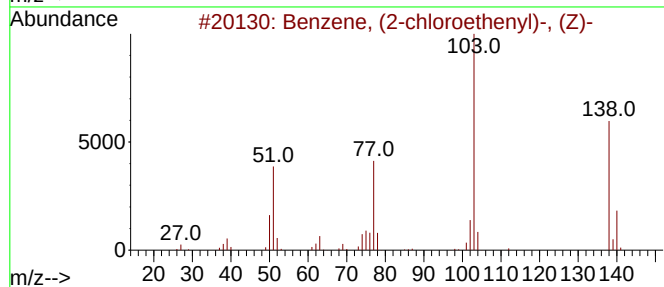
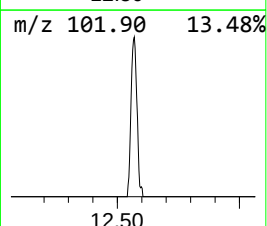
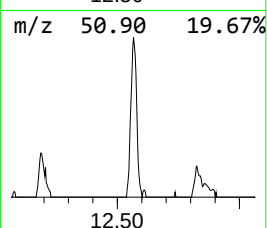
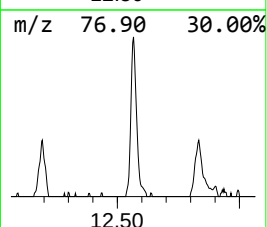
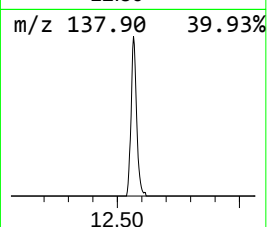
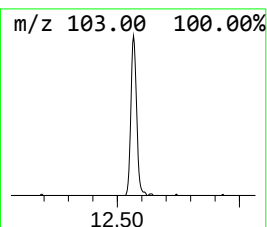
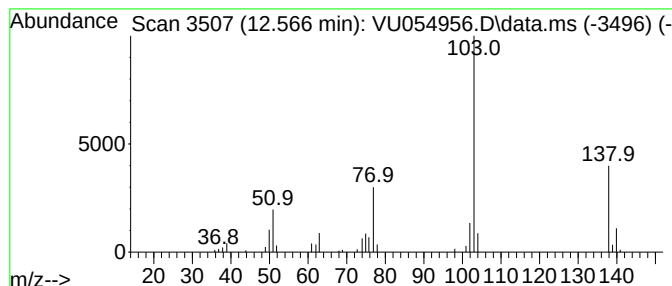
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR082823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Benzene, (2-chloroethenyl)-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.566	0.73 ug/L	83916	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-chloroethenyl)-, (Z)-	138	C8H7Cl	004604-28-8	94
2			Benzene, (2-chloroethenyl)-	138	C8H7Cl	000622-25-3	94
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	138	C8H7Cl	061599-88-0	93
4			Benzene, (2-chloroethenyl)-, (E)-	138	C8H7Cl	004110-77-4	91
5			Benzene, (1-chloroethenyl)-	138	C8H7Cl	000618-34-8	91



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Instrument :
MSVOA_U
ClientSampleId :
C0AR1

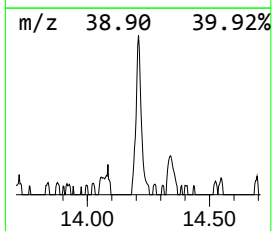
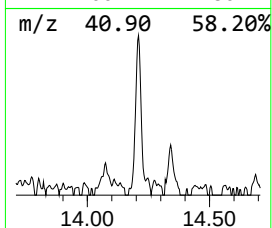
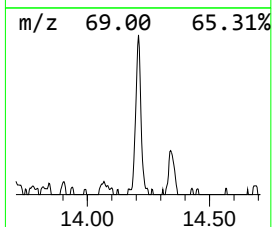
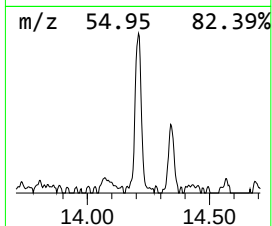
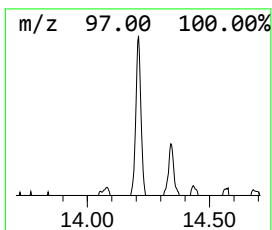
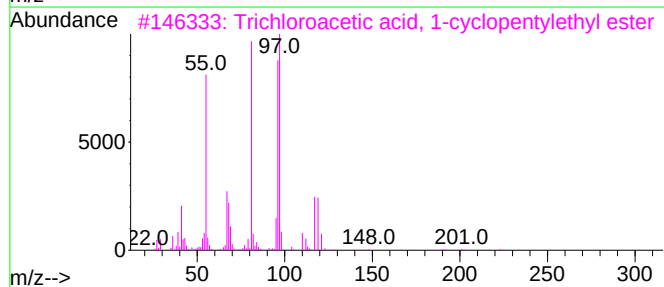
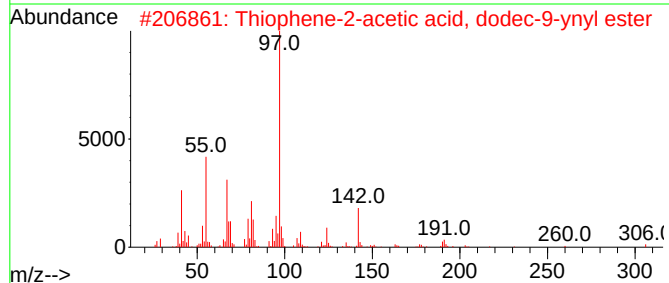
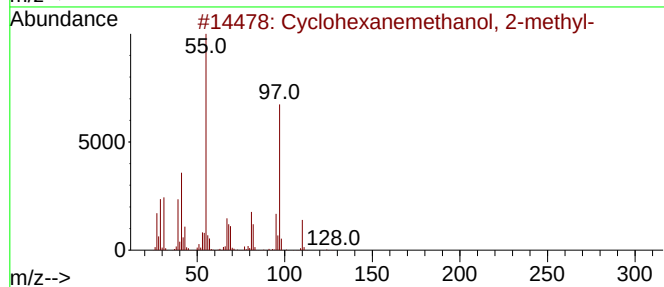
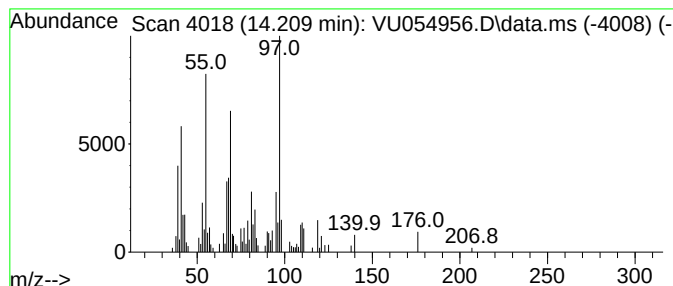
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR082823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Cyclohexanemethanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.209	0.58 ug/L	65831	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol, 2-methyl-	128	C8H16O	002105-40-0	50
2			Thiophene-2-acetic acid, dodec-9...	306	C18H26O2S	1000282-82-8	47
3			Trichloroacetic acid, 1-cyclopent...	258	C9H13Cl3O2	1000282-57-1	47
4			Cyclopentane, (1-methylbutyl)-	140	C10H20	004737-43-3	43
5			2-Pentene, 1-bromo-3,4-dimethyl-	176	C7H13Br	000922-99-6	43



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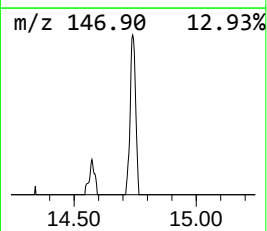
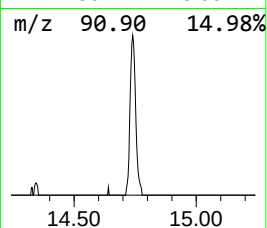
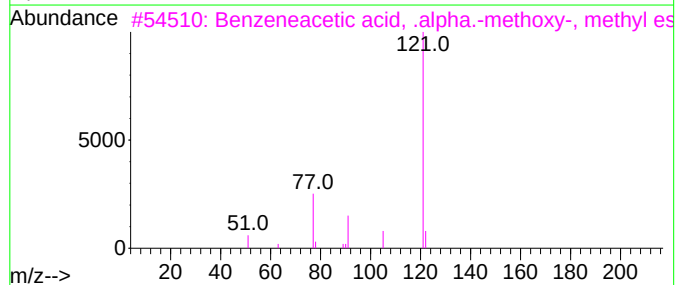
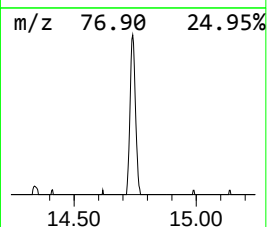
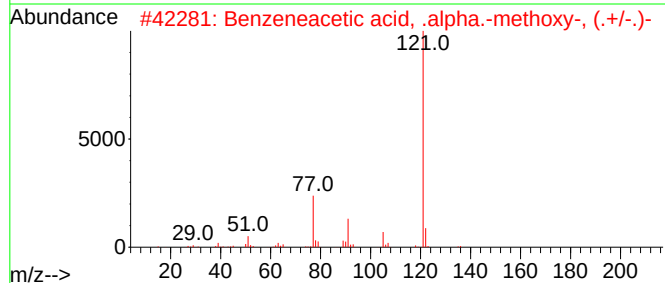
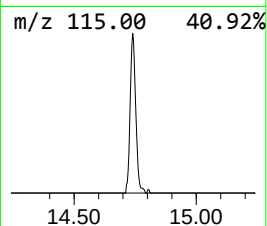
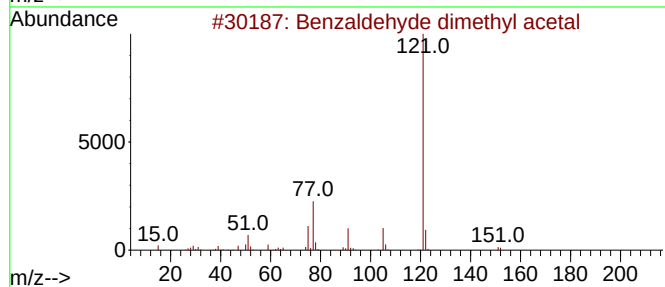
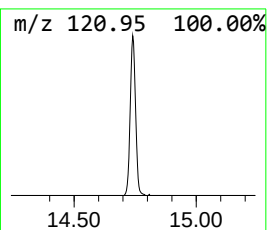
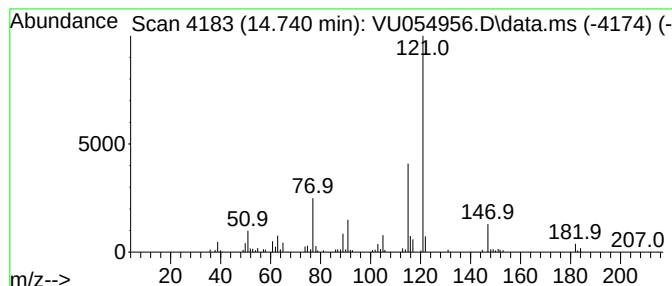
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR082823WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Benzaldehyde dimethyl acetal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.740	0.69 ug/L	78582	1,4-Dichlorobenzene-d4	11.811

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde dimethyl acetal	152	C9H12O2	001125-88-8	53
2			Benzeneacetic acid, .alpha.-meth...	166	C9H10O3	007021-09-2	47
3			Benzeneacetic acid, .alpha.-meth...	180	C10H12O3	056143-21-6	47
4			Benzeneacetic acid, .alpha.-meth...	180	C10H12O3	056143-21-6	47
5			(R)-(-)-.alpha.-Methoxyphenylace...	166	C9H10O3	003966-32-3	47



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, (2-chl...	12.566	0.7	ug/L	83916	3	11.811	571181	5.0
Cyclohexanemeth...	14.209	0.6	ug/L	65831	3	11.811	571181	5.0
Benzaldehyde di...	14.740	0.7	ug/L	78582	3	11.811	571181	5.0