

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV082423\
 Data File : VV031910.D
 Acq On : 24 Aug 2023 15:35
 Operator : SY/MD
 Sample : 04158-09
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 60 Sample Multiplier: 1

Instrument :
 MSVOA_V
 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_V\Method\SFAMVTR082323WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV031910.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.217	49	55	63	rBV2	5591	8233	1.77%	0.216%
2	1.278	69	74	82	rVB	26536	26837	5.78%	0.705%
3	1.359	93	99	108	rBV	9281	13108	2.82%	0.344%
4	1.536	147	154	170	rVB	33197	40740	8.78%	1.069%
5	2.063	309	318	329	rVB	58825	84196	18.14%	2.210%
6	2.452	431	439	451	rVB6	2820	5399	1.16%	0.142%
7	3.815	852	863	892	rBV2	47512	175343	37.78%	4.603%
8	4.256	984	1000	1027	rBV2	54248	144651	31.16%	3.797%
9	4.963	1204	1220	1243	rBV3	130662	338161	72.86%	8.877%
10	5.539	1388	1399	1426	rBV	125045	264029	56.88%	6.931%
11	5.838	1480	1492	1504	rBV5	6049	13502	2.91%	0.354%
12	5.995	1528	1541	1561	rBV	80140	172975	37.27%	4.541%
13	6.921	1818	1829	1847	rBV	35062	69394	14.95%	1.822%
14	7.182	1901	1910	1918	rBV6	2704	5046	1.09%	0.132%
15	7.249	1920	1931	1947	rVV	155149	281252	60.59%	7.383%
16	7.326	1947	1955	1976	rVB	16287	33990	7.32%	0.892%
17	7.564	2018	2029	2050	rBV2	20459	41723	8.99%	1.095%
18	8.034	2165	2175	2214	rBV	220546	464153	100.00%	12.185%
19	8.789	2399	2410	2430	rBV	188064	313911	67.63%	8.241%
20	9.349	2577	2584	2595	rBV2	4287	7618	1.64%	0.200%
21	9.509	2618	2634	2648	rBV6	7957	16738	3.61%	0.439%
22	10.159	2822	2836	2851	rBV	58822	94920	20.45%	2.492%
23	10.329	2879	2889	2896	rBV4	4390	6844	1.47%	0.180%
24	10.892	3049	3064	3087	rBV4	4497	15540	3.35%	0.408%
25	11.191	3145	3157	3183	rBV	215085	344760	74.28%	9.050%
26	11.503	3243	3254	3262	rBV4	7142	16544	3.56%	0.434%
27	11.564	3263	3273	3291	rVB	172501	280408	60.41%	7.361%
28	11.725	3315	3323	3334	rVB10	3662	6603	1.42%	0.173%
29	11.947	3382	3392	3407	rBV	65955	104443	22.50%	2.742%
30	12.204	3462	3472	3475	rBV3	3246	5307	1.14%	0.139%
31	12.593	3585	3593	3604	rBV3	13710	22520	4.85%	0.591%
32	12.712	3623	3630	3639	rBV7	4129	6138	1.32%	0.161%
33	12.841	3667	3670	3683	rVB7	3651	4737	1.02%	0.124%
34	13.583	3888	3901	3913	rBV3	30913	48342	10.42%	1.269%
35	13.715	3936	3942	3955	rVB3	9527	14292	3.08%	0.375%
36	13.992	4019	4028	4035	rBV3	3081	4839	1.04%	0.127%

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Title : TRACE VOA SFAM1.0

37	14.117	4056	4067	4081	rVV	40175	60904	13.12%	1.599%
38	15.953	4630	4638	4644	rBV9	4164	5957	1.28%	0.156%
39	15.985	4644	4648	4656	rVB6	4184	5290	1.14%	0.139%
40	16.213	4710	4719	4731	rBV2	14652	27093	5.84%	0.711%
41	16.426	4773	4785	4798	rBV	112919	186427	40.16%	4.894%
42	16.606	4834	4841	4848	rVB5	5445	8451	1.82%	0.222%
43	17.329	5058	5066	5074	rBV3	10397	18006	3.88%	0.473%

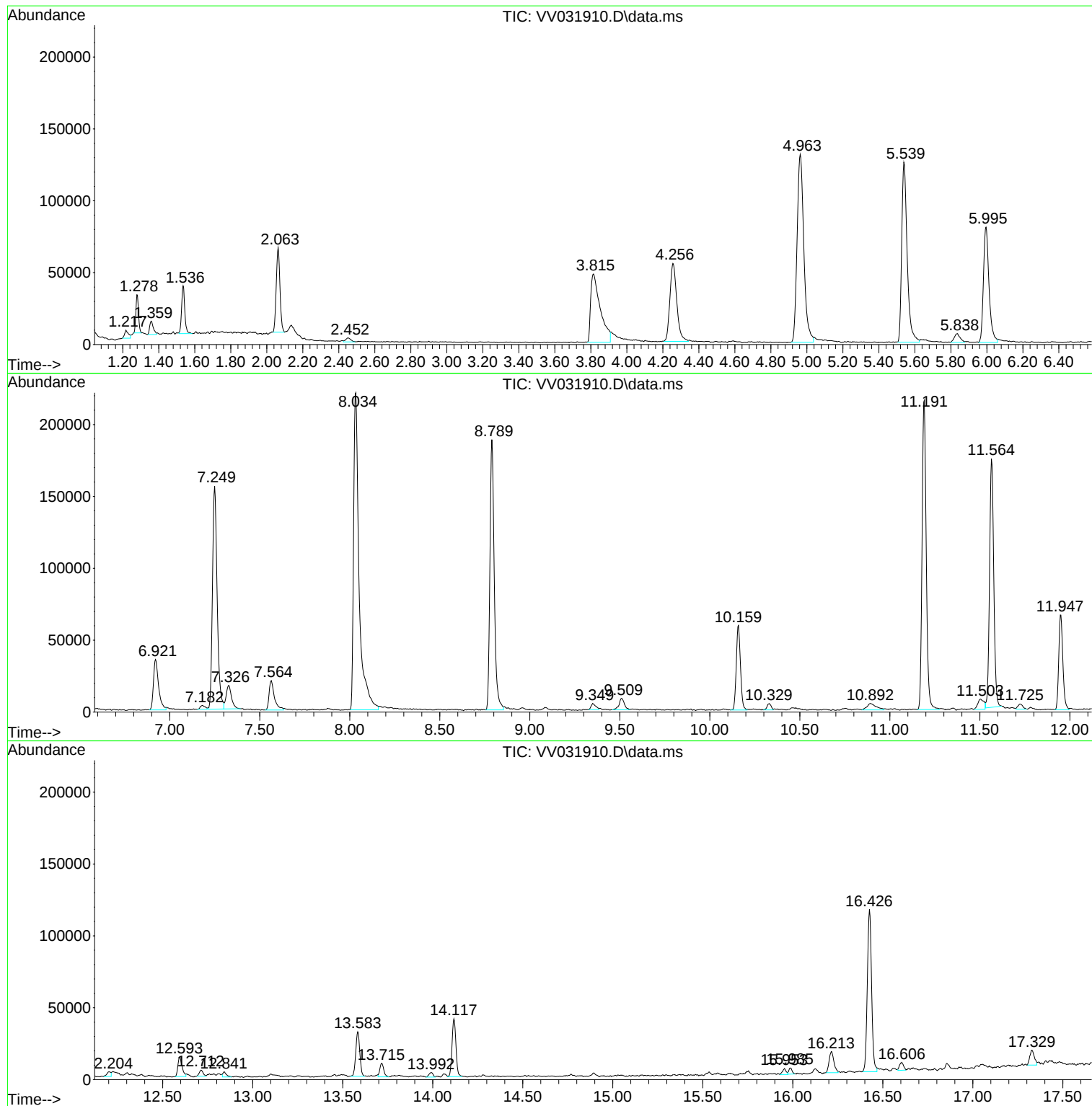
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Quant Title : TRACE VOA SFAM1.0

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



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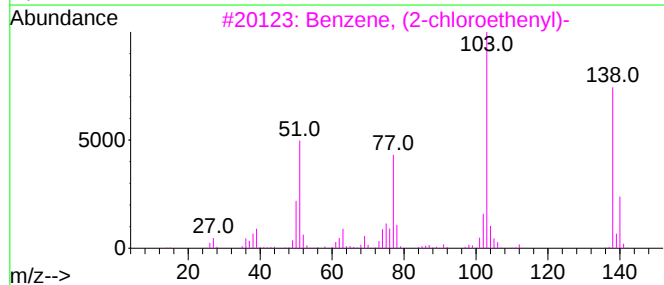
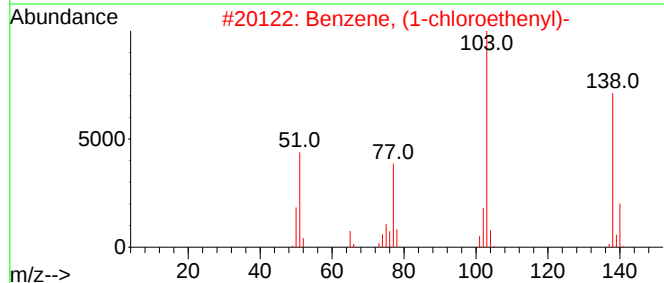
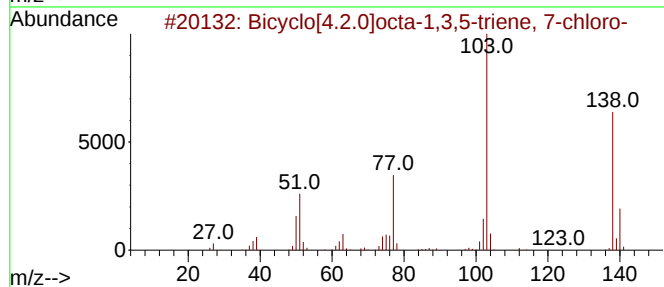
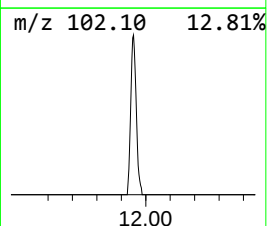
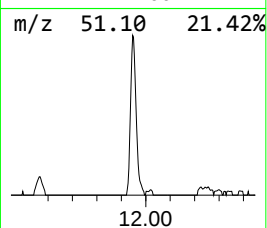
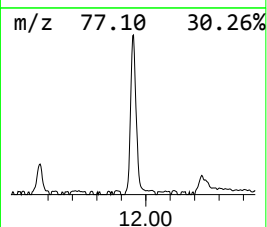
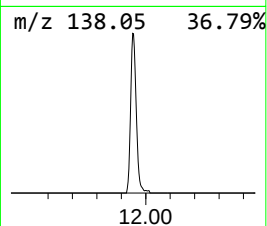
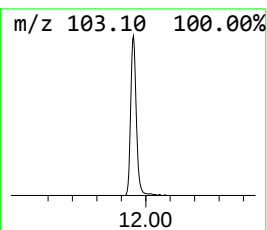
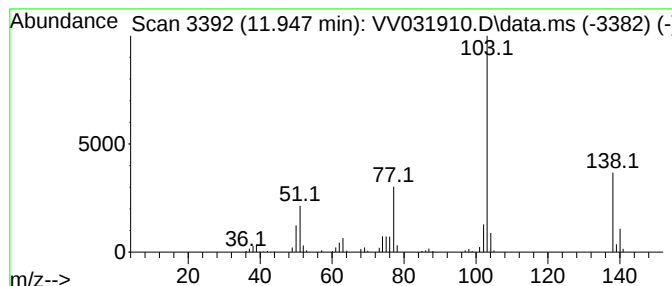
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR082323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.947	1.51 ug/L	104443	1,4-Dichlorobenzene-d4	11.191

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



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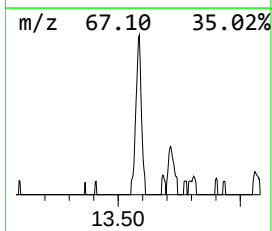
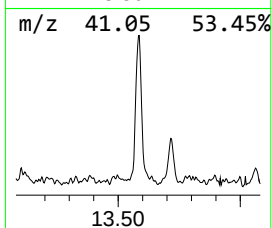
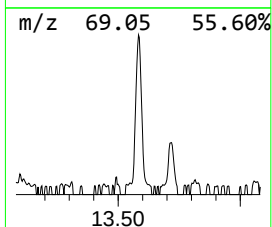
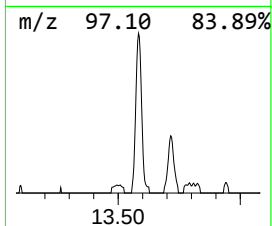
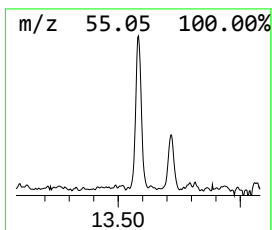
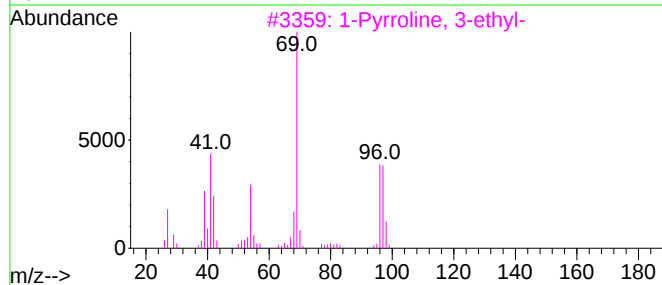
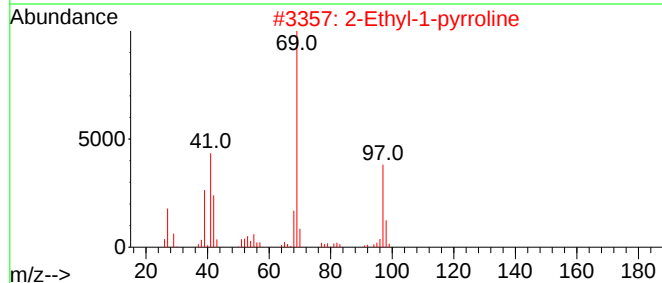
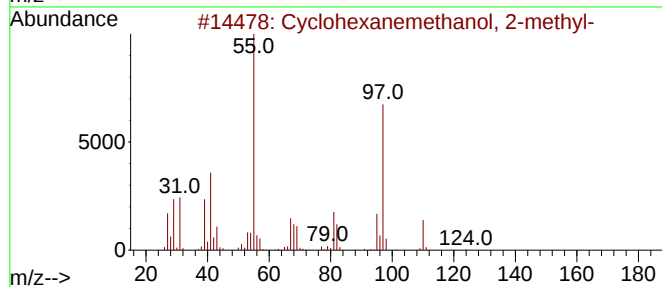
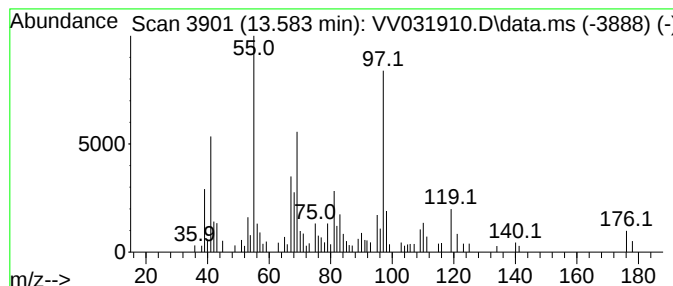
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR082323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Cyclohexanemethanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.583	0.70 ug/L	48342	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanemethanol, 2-methyl-	128	C8H16O	002105-40-0	50
2			2-Ethyl-1-pyrroline	97	C6H11N	1000422-81-4	49
3			1-Pyrroline, 3-ethyl-	97	C6H11N	1000073-06-0	47
4			Aziridine, 1-(1-butenyl)-, (E)-	97	C6H11N	080839-92-5	47
5			1-Methyl-3-piperidyl cyclopentyl...	317	C19H27NO3	1010289-59-7	38



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ClientSampleId :
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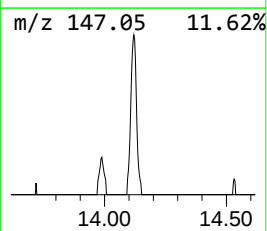
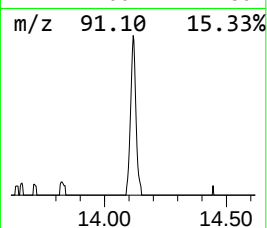
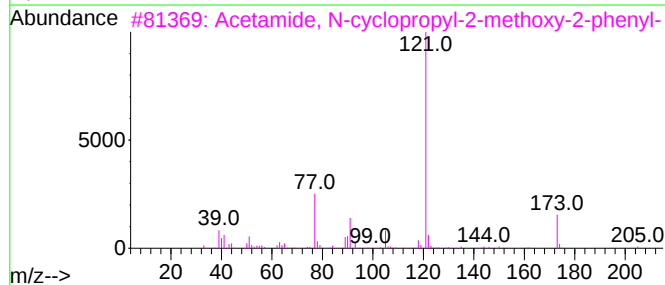
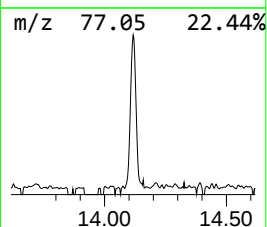
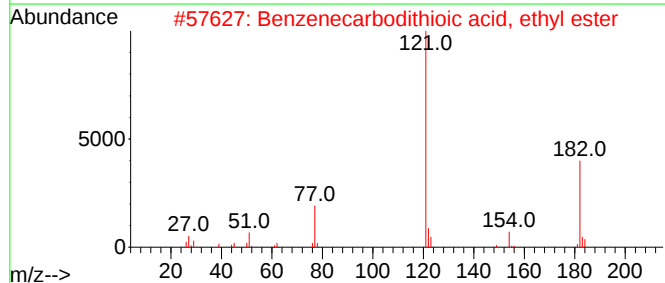
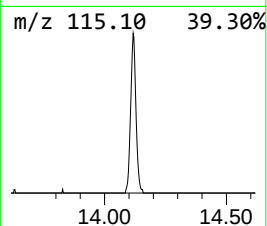
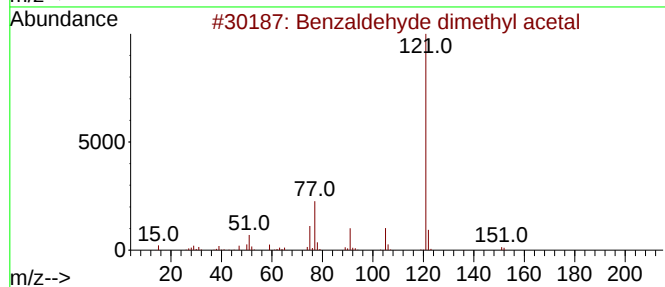
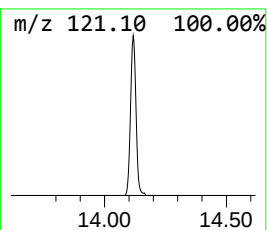
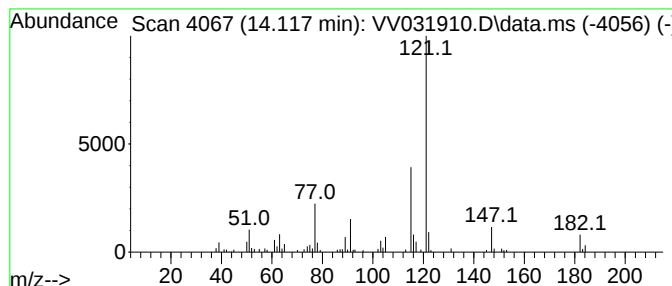
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR082323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.117	0.88 ug/L	60904	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde dimethyl acetal	152	C9H12O2	001125-88-8	49
2			Benzenecarbodithioic acid, ethyl...	182	C9H10S2	000936-63-0	47
3			Acetamide, N-cyclopropyl-2-metho...	205	C12H15NO2	1000305-01-6	47
4			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	47
5			2-(4-Methoxyphenyl)ethanol	152	C9H12O2	000702-23-8	47



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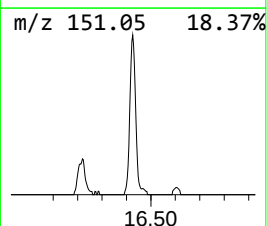
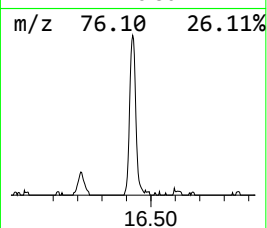
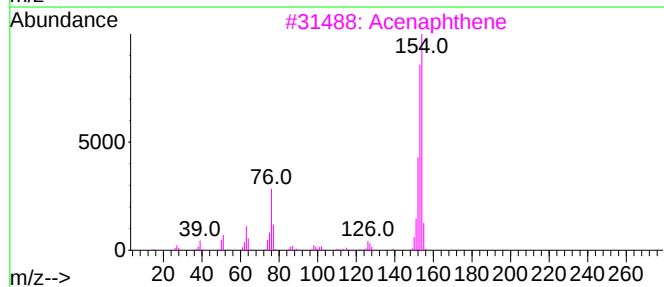
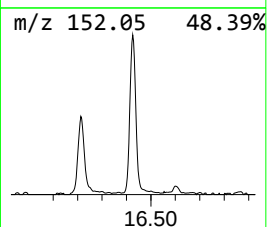
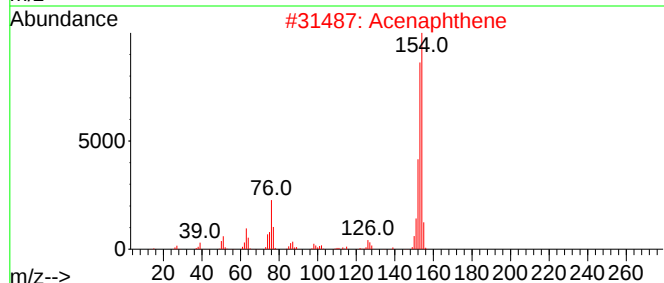
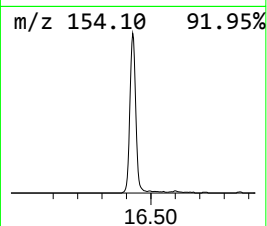
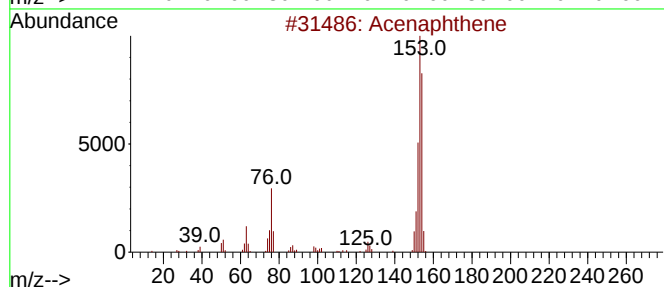
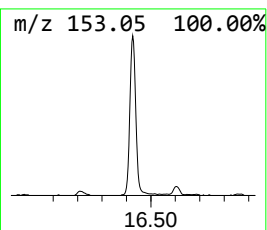
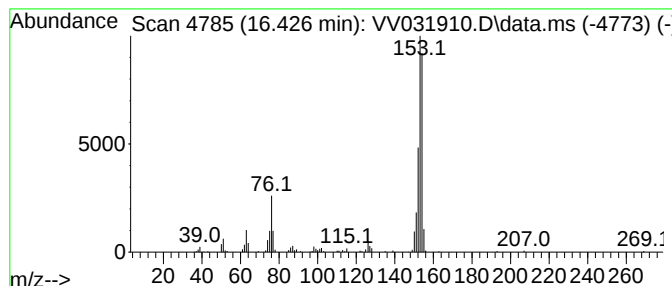
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexa-2,4-diyn-1-ylbenzene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.426	2.70 ug/L	186427	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	96
2			Acenaphthene	154	C12H10	000083-32-9	95
3			Acenaphthene	154	C12H10	000083-32-9	91
4			Acenaphthene	154	C12H10	000083-32-9	81
5			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	58



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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
Bicyclo[4.2.0]o...	11.947	1.5	ug/L	104443	3	11.191	344760	5.0
Cyclohexanemeth...	13.583	0.7	ug/L	48342	3	11.191	344760	5.0
unknown-01	14.117	0.9	ug/L	60904	3	11.191	344760	5.0
Hexa-2,4-diyne-1...	16.426	2.7	ug/L	186427	3	11.191	344760	5.0