

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111723\
 Data File : VU056432.D
 Acq On : 17 Nov 2023 11:10
 Operator : MD/SY
 Sample : 05389-02
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 YCGB5

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\SFAMUTR111323WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU056432.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	87	95	112	rVB	99240	115293	12.40%	1.262%
2	1.907	183	192	204	rBV	93637	125566	13.50%	1.374%
3	2.563	383	396	409	rBV	176609	288432	31.02%	3.156%
4	2.785	447	465	484	rBV3	10967	36319	3.91%	0.397%
5	3.039	535	544	557	rBV3	6313	11049	1.19%	0.121%
6	3.181	569	588	614	rBV2	17593	47504	5.11%	0.520%
7	4.615	1016	1034	1070	rBV	139733	369634	39.75%	4.045%
8	5.055	1157	1171	1198	rBV	184861	417142	44.86%	4.565%
9	5.721	1354	1378	1406	rBV2	349572	928438	99.84%	10.160%
10	6.245	1527	1541	1564	rBV	308729	598608	64.37%	6.551%
11	6.685	1665	1678	1706	rBV2	219439	440239	47.34%	4.818%
12	7.563	1935	1951	1971	rBV2	105892	192806	20.73%	2.110%
13	7.894	2040	2054	2084	rBV	405390	731969	78.72%	8.010%
14	8.177	2131	2142	2154	rBV	59975	104290	11.22%	1.141%
15	8.463	2219	2231	2243	rBV3	12866	24168	2.60%	0.264%
16	8.627	2271	2282	2318	rBV	487272	929887	100.00%	10.176%
17	9.412	2513	2526	2548	rBV	437973	766930	82.48%	8.393%
18	9.695	2603	2614	2628	rVB7	4986	10201	1.10%	0.112%
19	10.483	2846	2859	2876	rBV3	9429	17280	1.86%	0.189%
20	10.753	2930	2943	2957	rBV	150015	243337	26.17%	2.663%
21	10.888	2972	2985	3000	rVB2	24664	42548	4.58%	0.466%
22	11.290	3100	3110	3125	rVB2	24471	39813	4.28%	0.436%
23	11.807	3259	3271	3288	rBV	394695	662964	71.30%	7.255%
24	11.891	3289	3297	3307	rVB2	14919	24831	2.67%	0.272%
25	12.090	3345	3359	3377	rBV2	110397	178715	19.22%	1.956%
26	12.190	3377	3390	3406	rBV	406108	669990	72.05%	7.332%
27	12.479	3469	3480	3491	rVB7	9609	17335	1.86%	0.190%
28	12.611	3512	3521	3530	rVB4	9552	14049	1.51%	0.154%
29	12.679	3530	3542	3559	rBV4	50790	111285	11.97%	1.218%
30	12.871	3592	3602	3608	rBV5	11605	21111	2.27%	0.231%
31	12.923	3610	3618	3627	rVV2	35689	60648	6.52%	0.664%
32	12.968	3627	3632	3641	rVB4	9837	14264	1.53%	0.156%
33	13.035	3641	3653	3665	rBV9	9304	19433	2.09%	0.213%
34	13.109	3666	3676	3691	rVB2	28330	52004	5.59%	0.569%
35	13.322	3730	3742	3750	rVB4	6725	10207	1.10%	0.112%
36	13.447	3771	3781	3791	rVB6	21871	35279	3.79%	0.386%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	13.518	3794	3803	3813	rBV5	13158	22470	2.42%	0.246%
38	13.624	3822	3836	3851	rBV3	45824	78824	8.48%	0.863%
39	13.778	3876	3884	3892	rVV6	7940	12502	1.34%	0.137%
40	13.830	3892	3900	3909	rVV2	18465	30321	3.26%	0.332%
41	13.907	3909	3924	3927	rVV5	16863	31459	3.38%	0.344%
42	13.936	3928	3933	3948	rVB2	27123	50184	5.40%	0.549%
43	14.055	3960	3970	3977	rBV	92253	147855	15.90%	1.618%
44	14.103	3977	3985	3996	rVV5	73887	141077	15.17%	1.544%
45	14.174	3996	4007	4017	rVV6	26187	61620	6.63%	0.674%
46	14.235	4019	4026	4034	rVV3	16711	32950	3.54%	0.361%
47	14.283	4034	4041	4049	rVV5	19606	31631	3.40%	0.346%
48	14.338	4050	4058	4067	rVV7	12884	22888	2.46%	0.250%
49	14.392	4067	4075	4083	rVB5	10169	15484	1.67%	0.169%
50	14.482	4093	4103	4111	rBV6	7992	12819	1.38%	0.140%
51	14.553	4116	4125	4138	rVB6	6437	15349	1.65%	0.168%
52	15.167	4301	4316	4334	rVB3	22300	39762	4.28%	0.435%
53	15.428	4385	4397	4409	rBV4	8942	17246	1.85%	0.189%

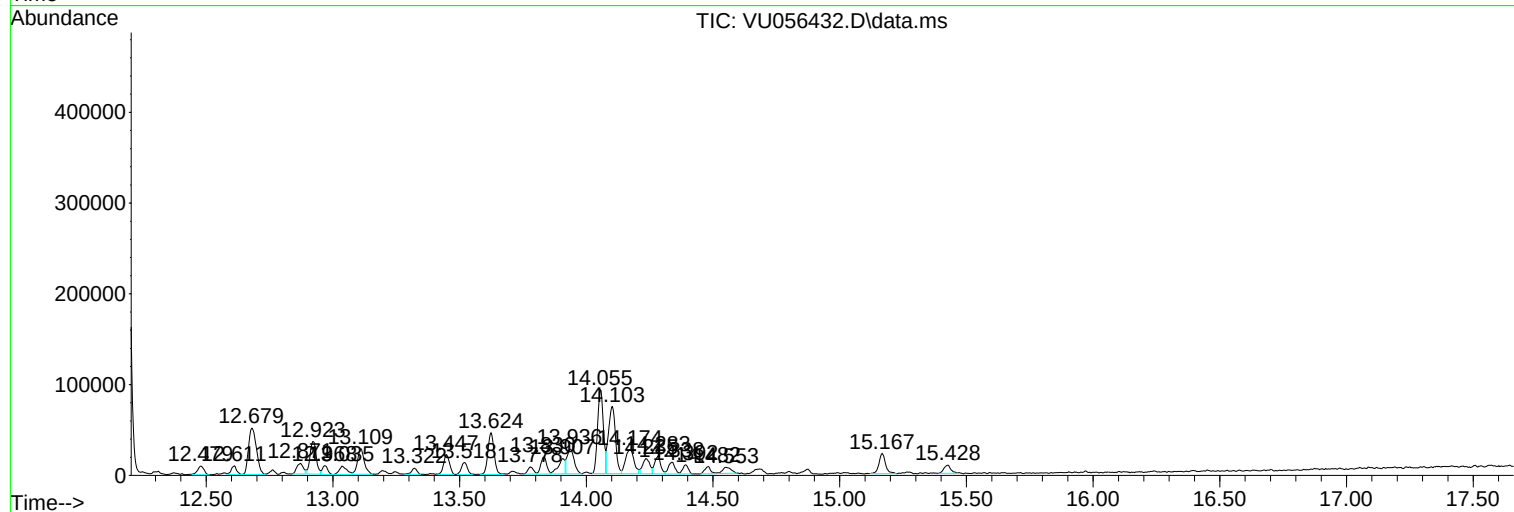
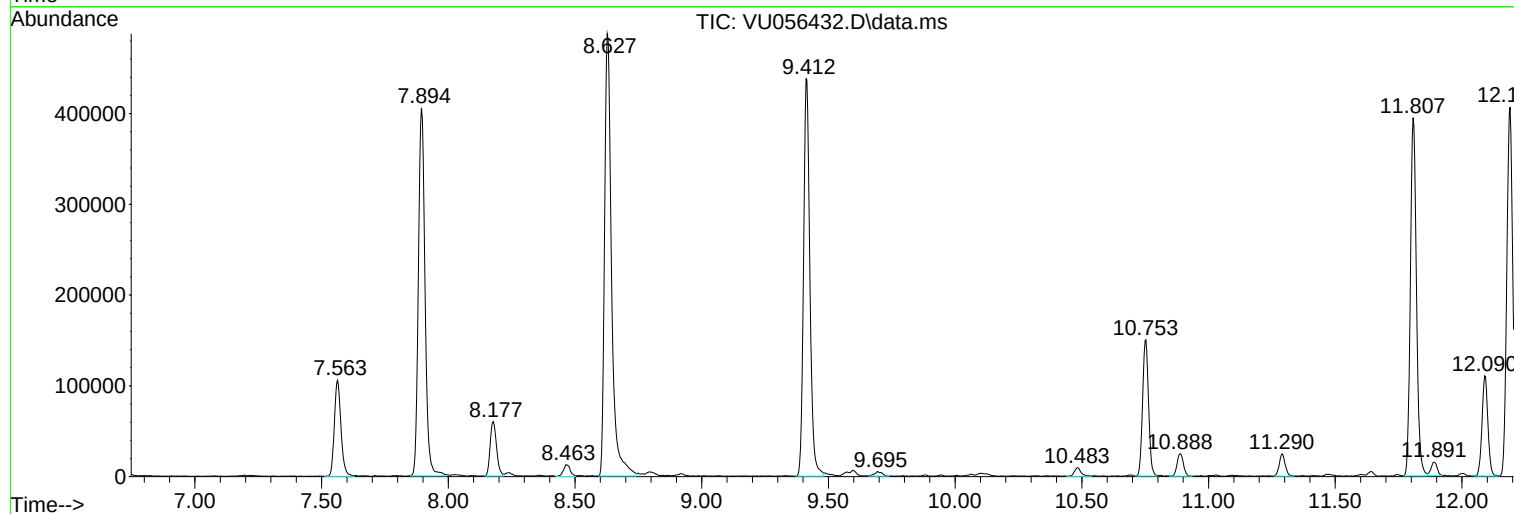
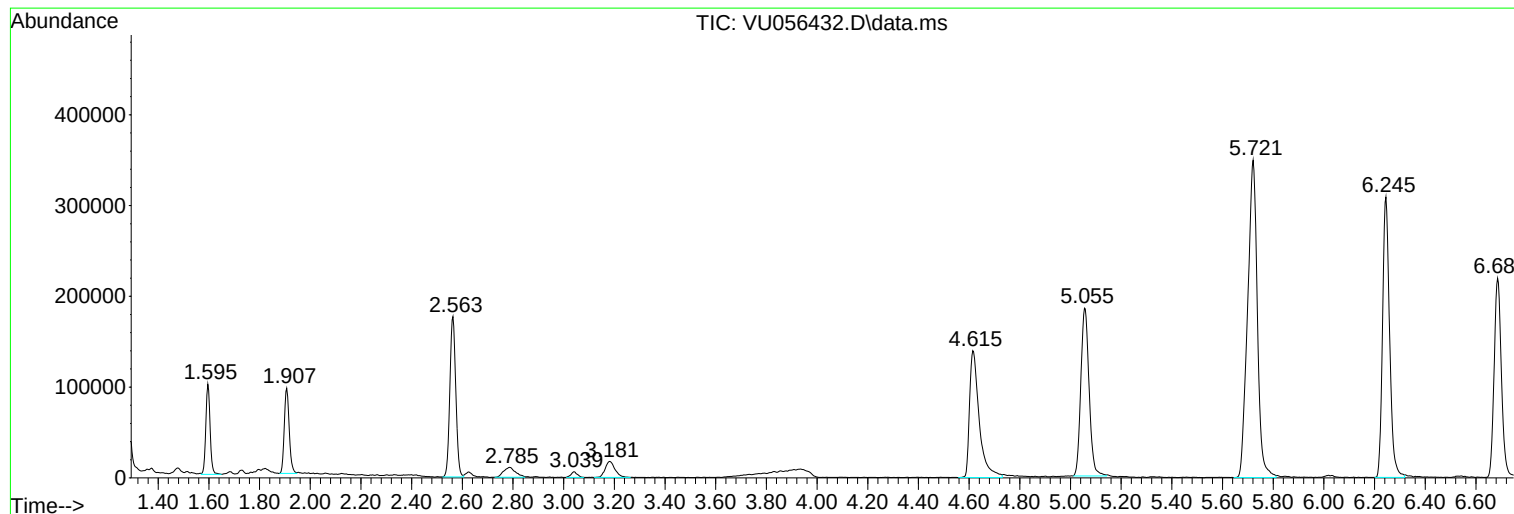
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Quant Title : TRACE VOA SFAM1.0

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



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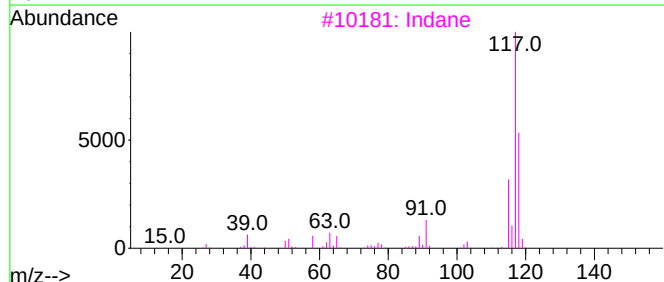
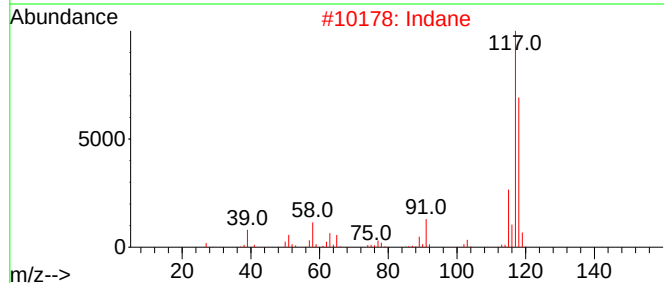
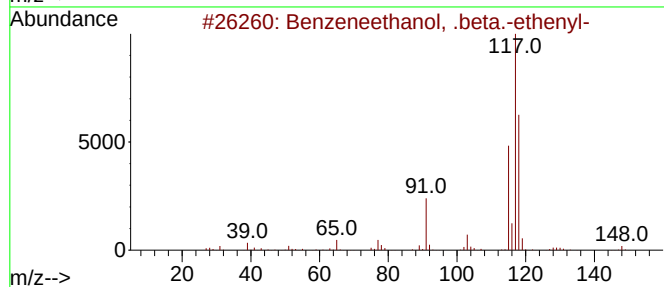
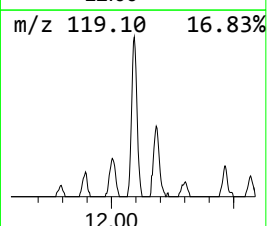
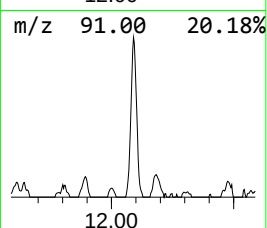
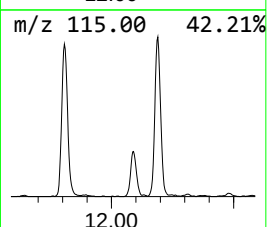
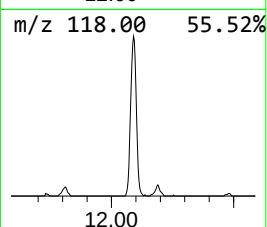
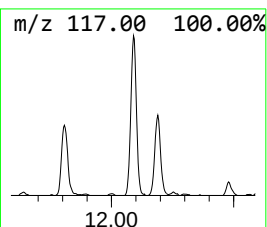
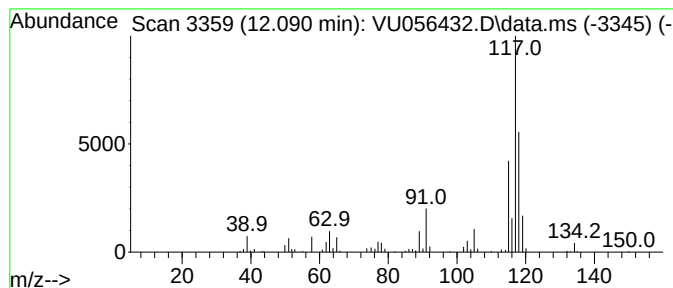
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Benzeneethanol, .beta.-ethe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.090	1.35 ug/L	178715	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	72
2			Indane	118	C9H10	000496-11-7	70
3			Indane	118	C9H10	000496-11-7	70
4			Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
5			Benzene, 2-propenyl-	118	C9H10	000300-57-2	64



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Misc : 25mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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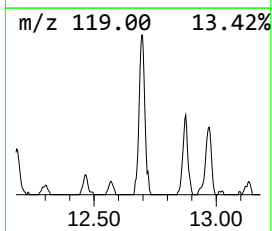
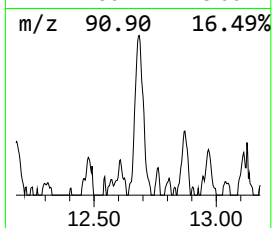
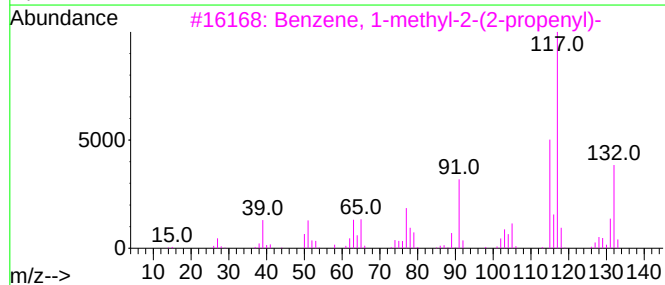
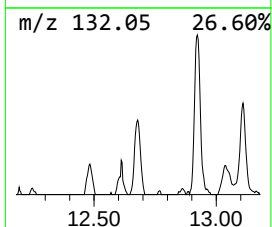
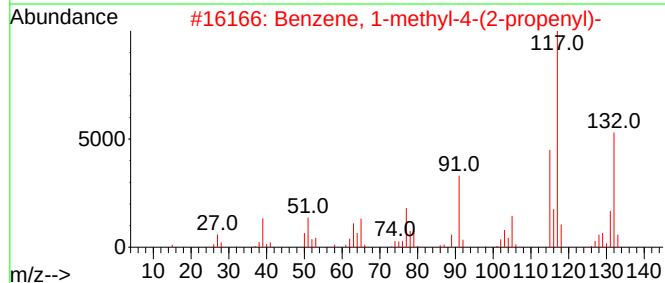
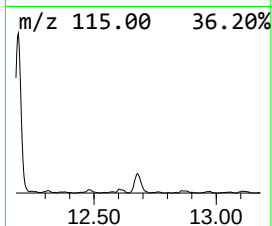
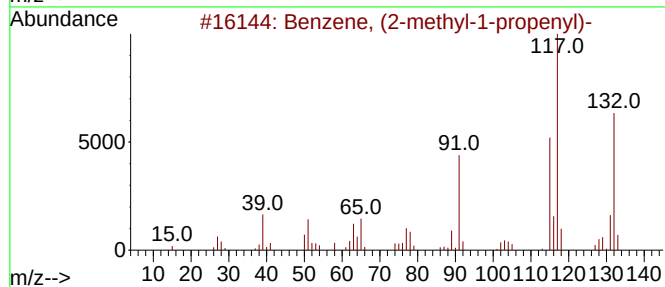
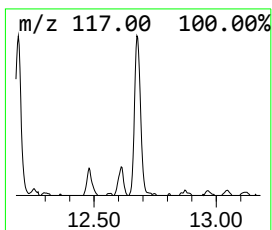
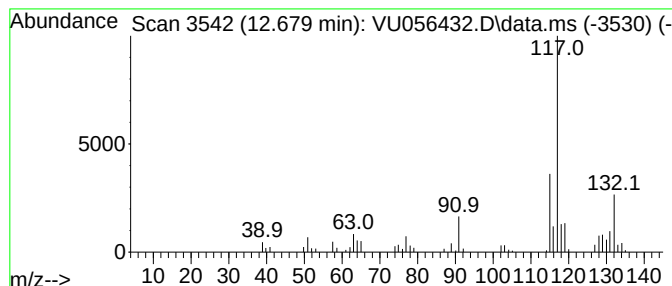
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Benzene, (2-methyl-1-propen... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.679	0.84 ug/L	111285	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
2			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	87
3			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	83
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	83
5			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	83



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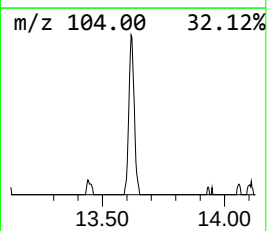
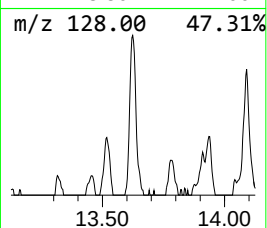
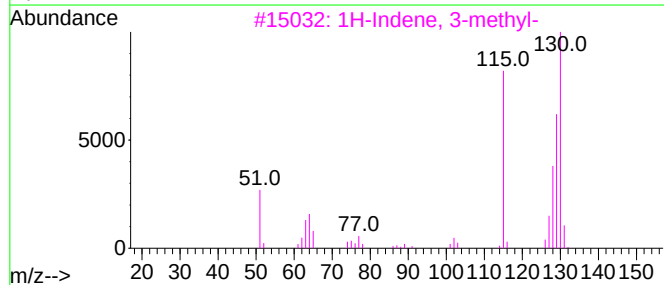
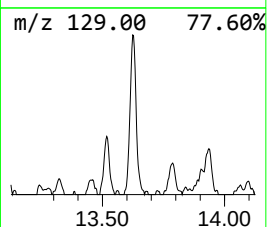
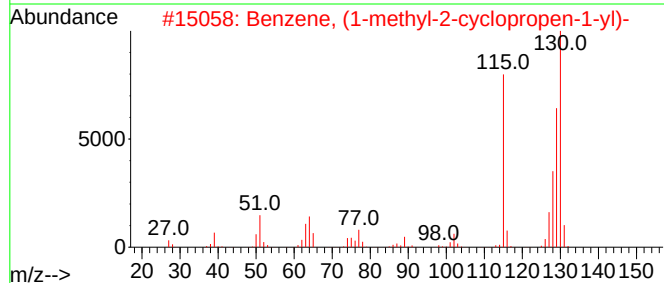
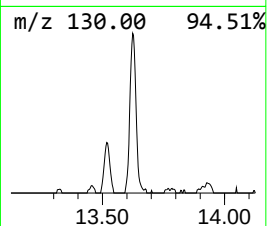
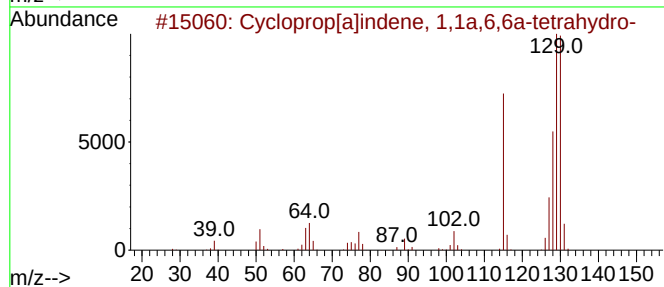
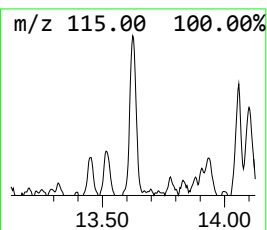
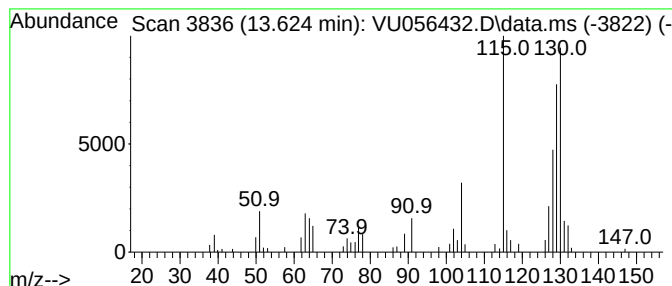
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Cycloprop[a]indene, 1,1a,6,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.624	0.59 ug/L	78824	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	96
2			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	96
3			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	95
4			Benzene,1-methyl-1,2-propadienyl-	130	C10H10	022433-39-2	95
5			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	95



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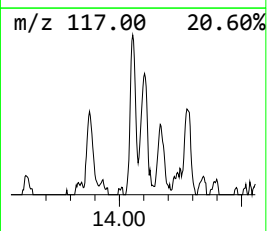
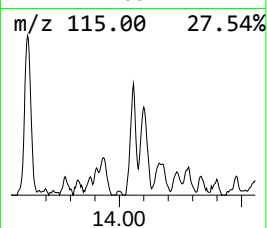
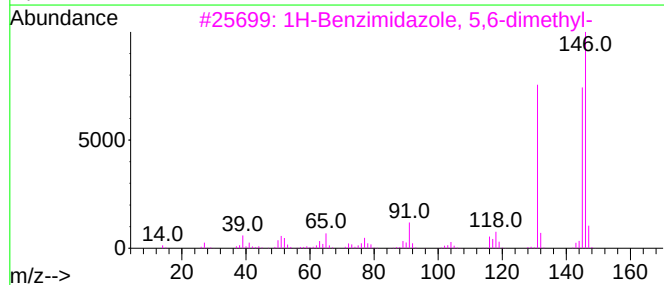
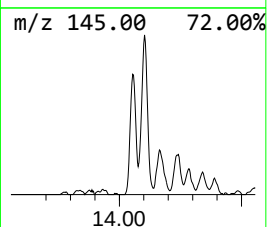
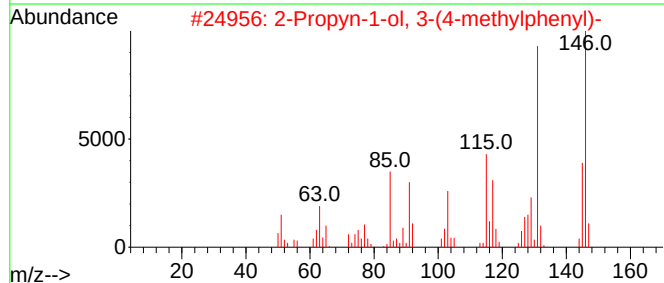
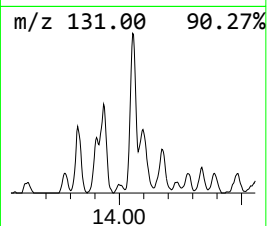
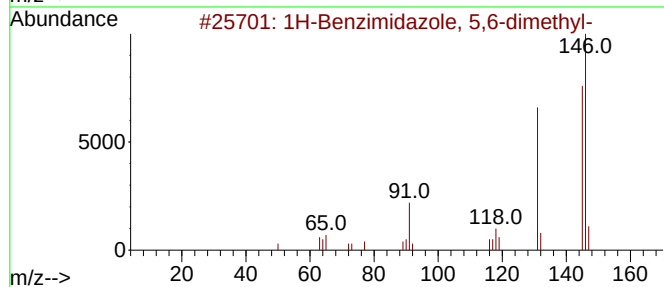
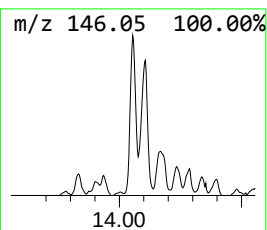
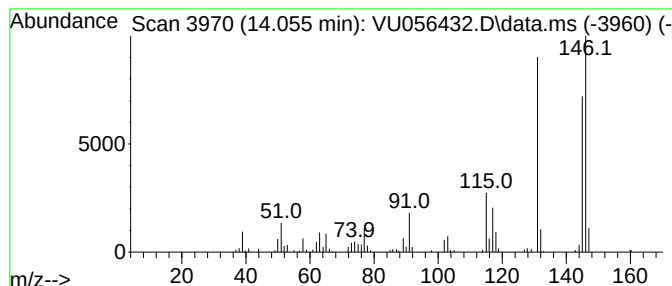
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1H-Benzimidazole, 5,6-dimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.055	1.12 ug/L	147855	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	87
2			2-Propyn-1-ol, 3-(4-methylphenyl)-	146	C10H10O	016017-24-6	87
3			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	83
4			1H-Inden-1-one, 2,3-dihydro-2-me...	146	C10H10O	017496-14-9	80
5			Naphthalene, 1,2,3,4-tetrahydro-...	146	C11H14	002809-64-5	72



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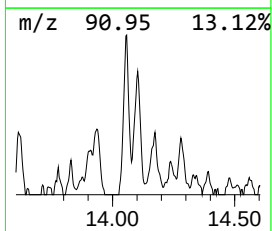
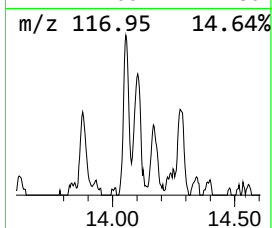
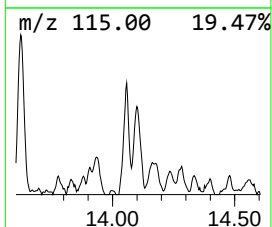
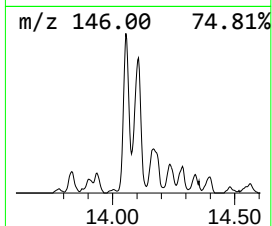
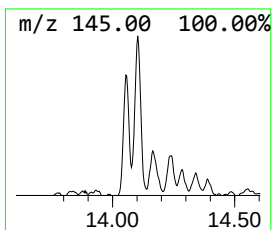
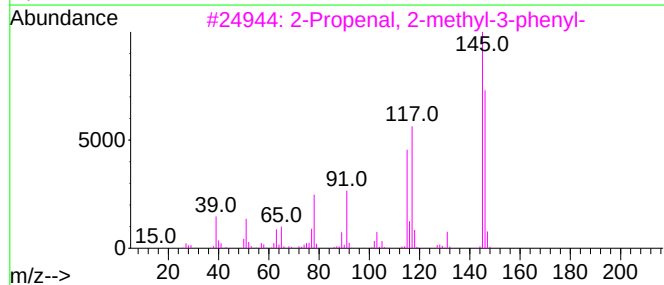
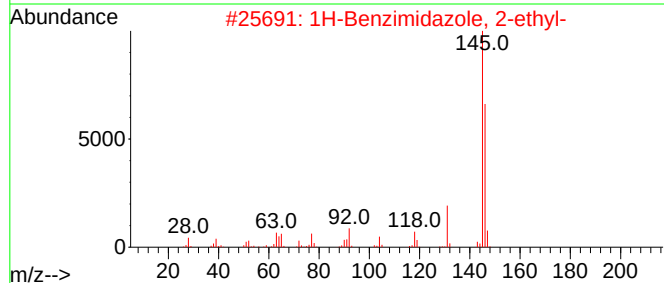
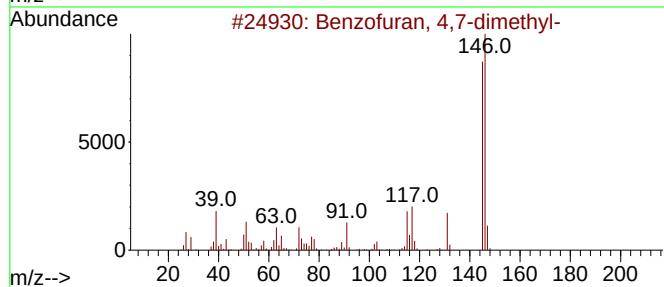
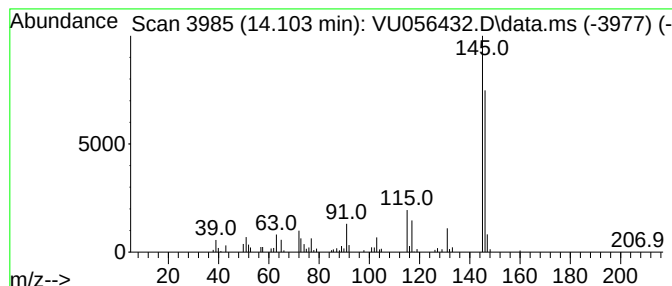
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Benzofuran, 4,7-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.103	1.06 ug/L	141077	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	76
2			1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	64
3			2-Propenal, 2-methyl-3-phenyl-	146	C10H10O	000101-39-3	64
4			Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	59
5			7-Azaindole-3-carboxaldehyde	146	C8H6N2O	004649-09-6	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111723\
Data File : VU056432.D
Acq On : 17 Nov 2023 11:10
Operator : MD/SY
Sample : 05389-02
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YCGB5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
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
Benzeneethanol,...	12.090	1.4	ug/L	178715	3	11.807	662964	5.0
Benzene, (2-met...	12.679	0.8	ug/L	111285	3	11.807	662964	5.0
Cycloprop[a]ind...	13.624	0.6	ug/L	78824	3	11.807	662964	5.0
1H-Benzimidazol...	14.055	1.1	ug/L	147855	3	11.807	662964	5.0
Benzofuran, 4,7...	14.103	1.1	ug/L	141077	3	11.807	662964	5.0