

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111723\
 Data File : VU056439.D
 Acq On : 17 Nov 2023 14:01
 Operator : MD/SY
 Sample : 05389-12
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 YCGB9

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: VU056439.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	87	95	105	rBV	93677	106878	11.36%	1.246%
2	1.727	130	136	143	rBV	8692	9740	1.04%	0.114%
3	1.904	182	191	204	rBV	90952	123989	13.18%	1.446%
4	2.560	383	395	409	rBV	170293	276436	29.38%	3.223%
5	3.042	533	545	555	rBV3	5030	9700	1.03%	0.113%
6	3.181	575	588	606	rVB2	8756	21185	2.25%	0.247%
7	4.615	1023	1034	1072	rBV	128716	331235	35.21%	3.862%
8	5.055	1155	1171	1200	rVB	173235	392224	41.69%	4.573%
9	5.721	1355	1378	1410	rBV3	352137	940769	100.00%	10.968%
10	6.245	1528	1541	1565	rBV	310533	602161	64.01%	7.020%
11	6.685	1664	1678	1702	rBV	218781	430794	45.79%	5.023%
12	7.563	1939	1951	1970	rBV	99528	176446	18.76%	2.057%
13	7.894	2041	2054	2076	rBV	401295	715648	76.07%	8.344%
14	8.177	2131	2142	2155	rBV2	60640	105953	11.26%	1.235%
15	8.627	2271	2282	2323	rBV	497020	924261	98.25%	10.776%
16	8.920	2363	2373	2384	rBV2	11991	18831	2.00%	0.220%
17	9.412	2512	2526	2560	rBV	434624	757582	80.53%	8.833%
18	9.569	2565	2575	2599	rVB4	7833	20219	2.15%	0.236%
19	10.753	2932	2943	2955	rBV	160705	259273	27.56%	3.023%
20	11.290	3100	3110	3124	rBV2	14375	23824	2.53%	0.278%
21	11.807	3258	3271	3289	rBV	413047	682673	72.57%	7.959%
22	11.891	3289	3297	3307	rVB2	9235	14561	1.55%	0.170%
23	12.094	3348	3360	3372	rBV4	36979	61241	6.51%	0.714%
24	12.190	3376	3390	3408	rBV	410654	678367	72.11%	7.909%
25	12.483	3470	3481	3490	rVB8	6252	10633	1.13%	0.124%
26	12.679	3531	3542	3560	rBV3	27786	58669	6.24%	0.684%
27	12.868	3590	3601	3607	rBV8	5436	9990	1.06%	0.116%
28	12.923	3611	3618	3629	rVB2	16634	26729	2.84%	0.312%
29	13.113	3668	3677	3686	rVB3	10859	17509	1.86%	0.204%
30	13.447	3772	3781	3793	rBV7	7581	11788	1.25%	0.137%
31	13.518	3793	3803	3816	rBV6	14123	23059	2.45%	0.269%
32	13.624	3826	3836	3848	rBV6	22236	37072	3.94%	0.432%
33	13.782	3875	3885	3893	rBV7	6570	11403	1.21%	0.133%
34	13.833	3893	3901	3909	rBV3	11866	17846	1.90%	0.208%
35	13.936	3927	3933	3943	rVB2	19993	31928	3.39%	0.372%
36	14.055	3959	3970	3978	rBV	102935	164061	17.44%	1.913%

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37	14.100	3978	3984	3996	rVV4	58473	108943	11.58%	1.270%
38	14.164	3996	4004	4018	rVV6	33072	77082	8.19%	0.899%
39	14.235	4018	4026	4034	rVV3	29305	52478	5.58%	0.612%
40	14.283	4034	4041	4050	rVV4	32542	50991	5.42%	0.594%
41	14.338	4050	4058	4067	rVV3	15381	25241	2.68%	0.294%
42	14.389	4067	4074	4083	rVB5	13903	19404	2.06%	0.226%
43	14.550	4109	4124	4129	rBV10	8701	18539	1.97%	0.216%
44	14.675	4151	4163	4173	rBV8	13911	27742	2.95%	0.323%
45	14.801	4193	4202	4211	rBV4	13760	21592	2.30%	0.252%
46	14.868	4213	4223	4234	rVB6	7398	15837	1.68%	0.185%
47	15.167	4302	4316	4334	rVB3	19140	39041	4.15%	0.455%
48	15.428	4385	4397	4402	rBV8	8508	15627	1.66%	0.182%

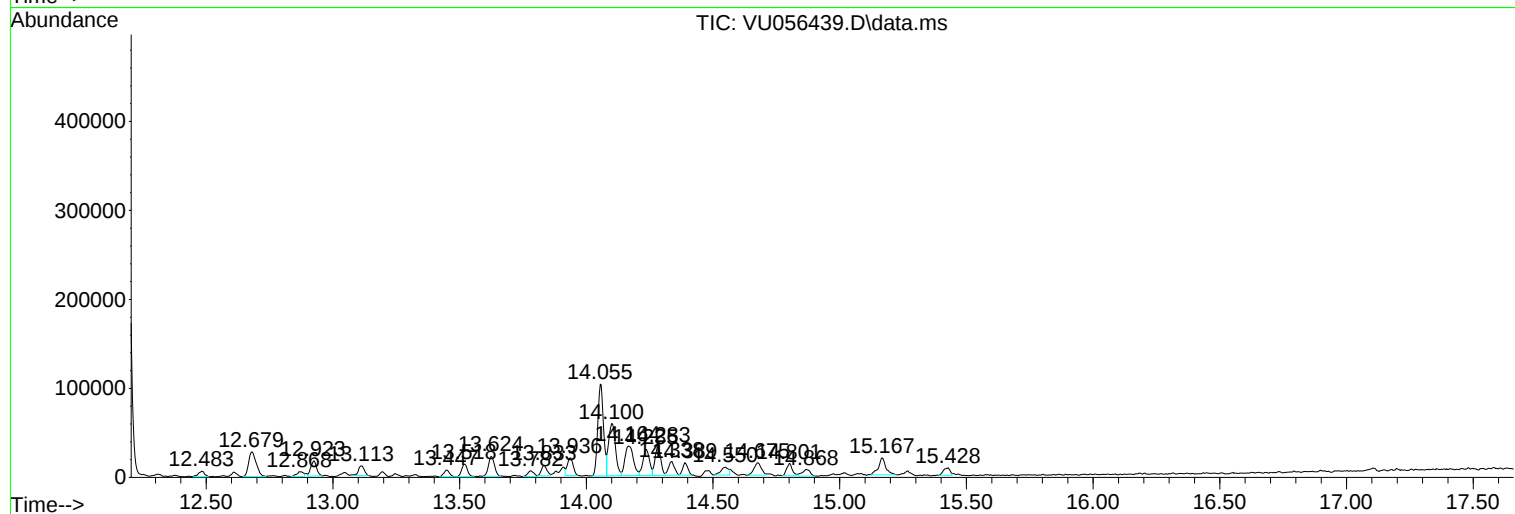
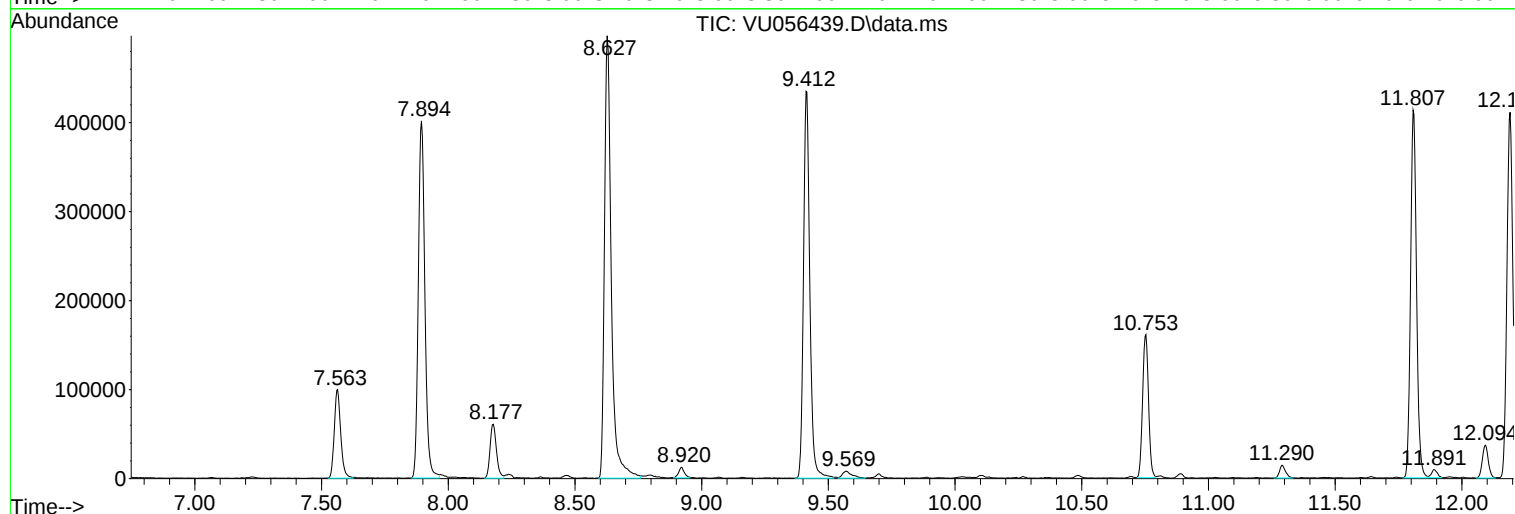
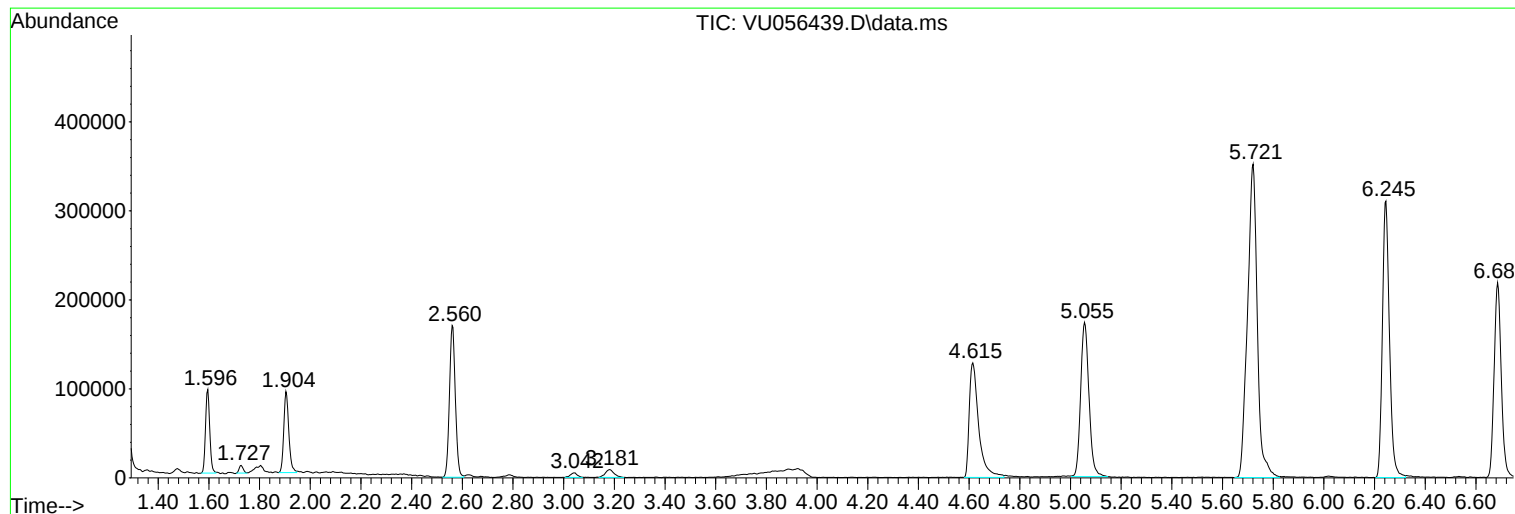
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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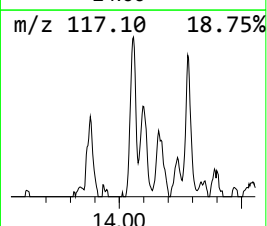
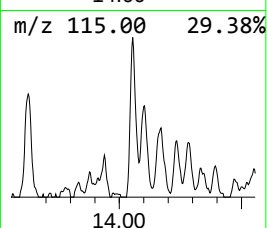
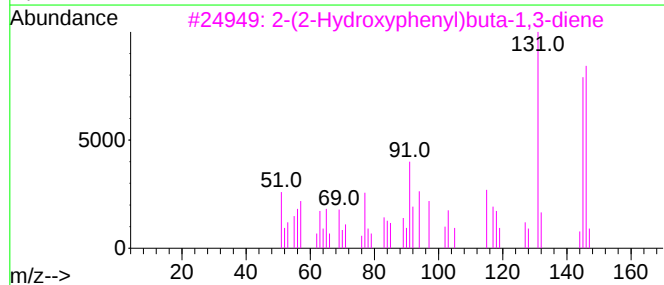
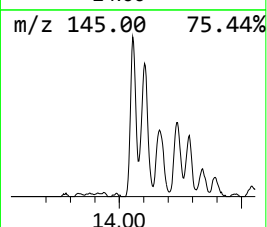
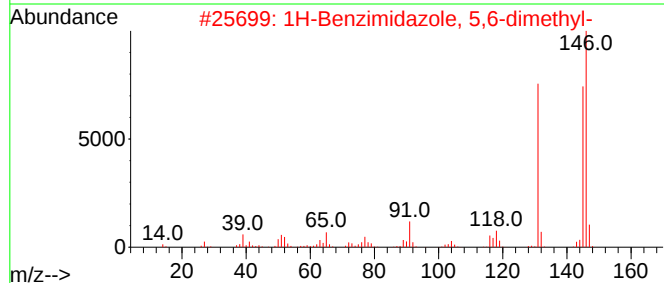
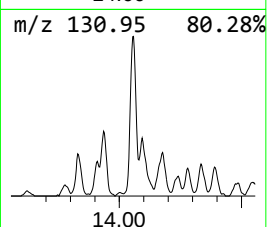
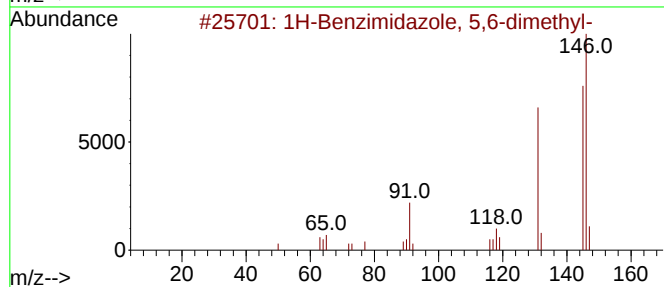
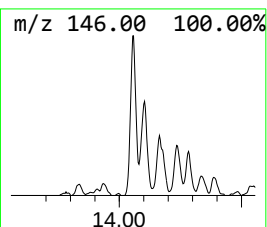
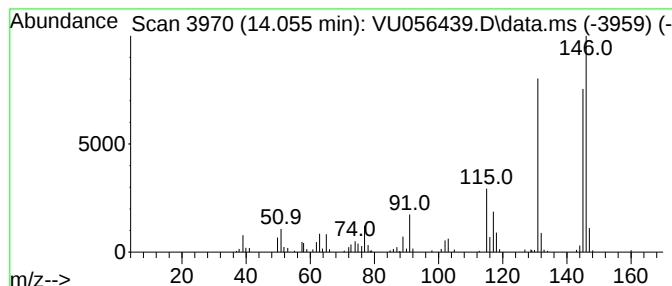
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 1H-Benzimidazole, 5,6-dimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.055	1.20 ug/L	164061	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	90
2			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	87
3			2-(2-Hydroxyphenyl)buta-1,3-diene	146	C10H10O	038865-47-3	86
4			1H-Indazole, 5,7-dimethyl-	146	C9H10N2	043067-41-0	83
5			3-Buten-2-one, 4-phenyl-	146	C10H10O	000122-57-6	72



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Instrument :
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YCGB9

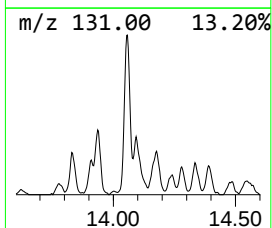
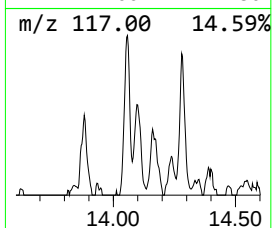
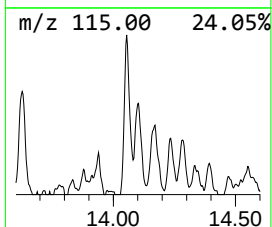
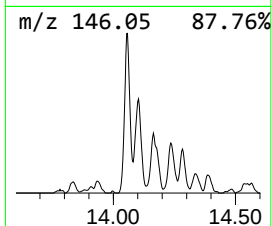
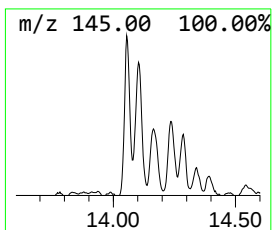
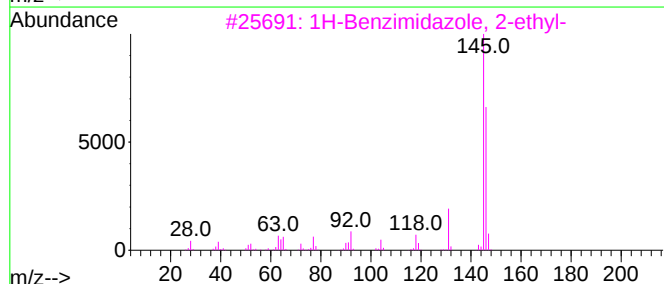
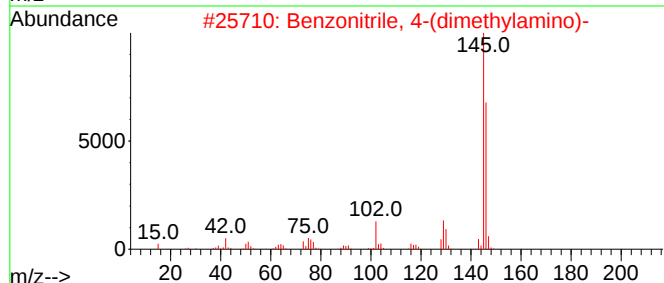
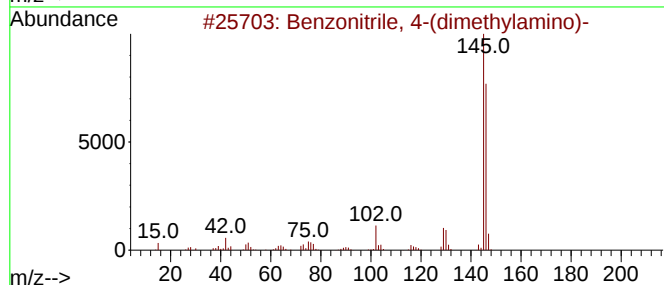
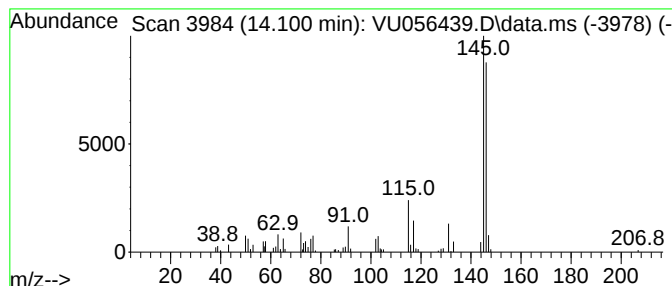
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Benzonitrile, 4-(dimethylam... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.100	0.80 ug/L	108943	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	64
2			Benzonitrile, 4-(dimethylamino)-	146	C9H10N2	001197-19-9	59
3			1H-Benzimidazole, 2-ethyl-	146	C9H10N2	001848-84-6	59
4			2,3-Dimethyl-1H-pyrrolo[2,3-b]py...	146	C9H10N2	010299-69-1	58
5			Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	53



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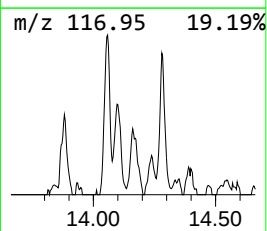
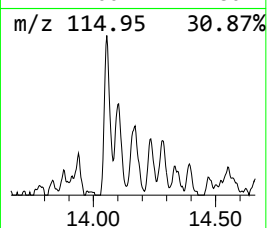
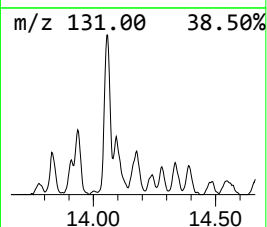
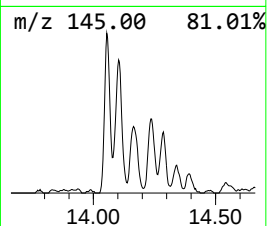
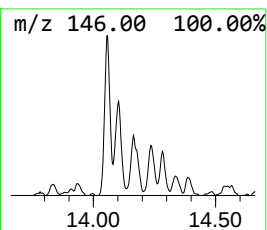
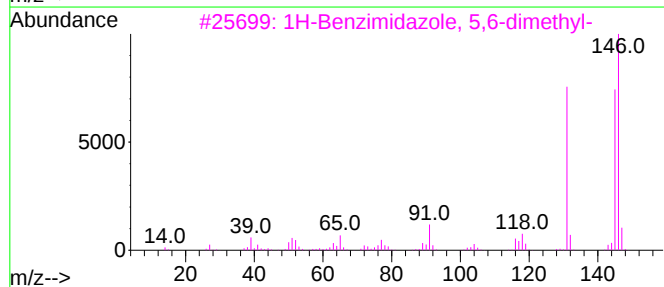
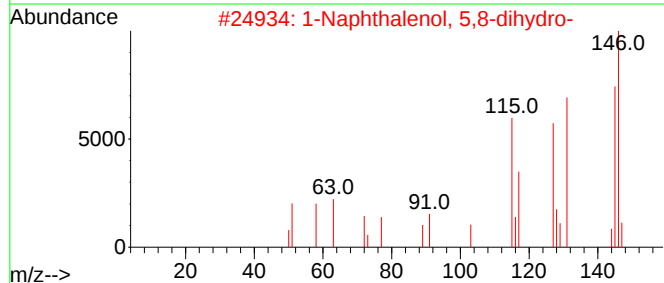
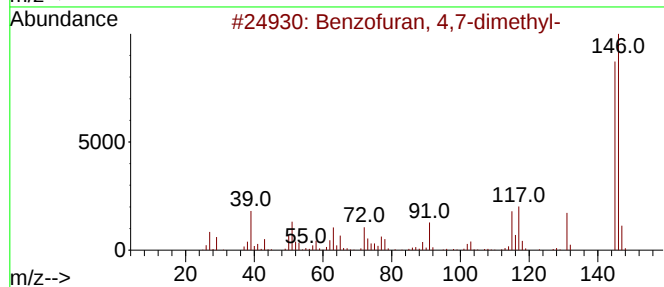
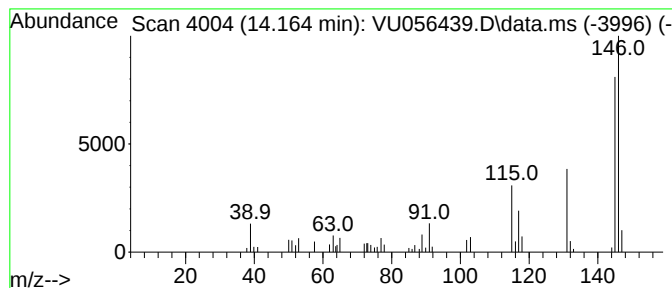
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.164	0.56 ug/L	77082	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzofuran, 4,7-dimethyl-	146	C10H10O	028715-26-6	74
2			1-Naphthalenol, 5,8-dihydro-	146	C10H10O	027673-48-9	72
3			1H-Benzimidazole, 5,6-dimethyl-	146	C9H10N2	000582-60-5	64
4			Imidazo[1,2-a]pyridine-3-carbal...	146	C8H6N2O	006188-43-8	62
5			1H-Indazole, 3,6-dimethyl-	146	C9H10N2	007746-28-3	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1H-Benzimidazol...	14.055	1.2	ug/L	164061	3	11.810	682673	5.0
Benzonitrile, 4...	14.100	0.8	ug/L	108943	3	11.810	682673	5.0
Benzofuran, 4,7...	14.164	0.6	ug/L	77082	3	11.810	682673	5.0