

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121623\
 Data File : VU056956.D
 Acq On : 17 Dec 2023 05:06
 Operator : MD/SY
 Sample : 05811-15
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F7B40

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: VU056956.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.470	50	56	64	rBV2	8939	11489	1.09%	0.099%
2	1.596	87	95	105	rVB	98555	111522	10.55%	0.963%
3	1.647	105	111	117	rBV	20064	23054	2.18%	0.199%
4	1.727	132	136	147	rVB2	8646	11146	1.05%	0.096%
5	1.911	185	193	210	rVB	83486	122758	11.62%	1.060%
6	1.994	211	219	230	rVB2	24426	35413	3.35%	0.306%
7	2.563	383	396	421	rBV2	159604	325673	30.82%	2.813%
8	3.036	529	543	564	rBV2	39562	85828	8.12%	0.741%
9	3.358	631	643	652	rBV5	6168	13528	1.28%	0.117%
10	3.846	786	795	808	rBV3	12175	29392	2.78%	0.254%
11	4.631	1028	1039	1077	rBV	96361	329327	31.17%	2.845%
12	5.055	1155	1171	1195	rBV	172631	388048	36.72%	3.352%
13	5.454	1282	1295	1311	rVB7	8358	19417	1.84%	0.168%
14	5.628	1336	1349	1359	rBV8	5445	11024	1.04%	0.095%
15	5.721	1359	1378	1407	rVV2	306304	830142	78.56%	7.171%
16	5.843	1408	1416	1428	rVV8	8766	19503	1.85%	0.168%
17	5.914	1428	1438	1451	rVB7	6030	12600	1.19%	0.109%
18	6.242	1527	1540	1570	rBV	330944	653606	61.85%	5.646%
19	6.685	1663	1678	1711	rBV	202592	414603	39.24%	3.582%
20	7.068	1785	1797	1817	rVB6	6018	11984	1.13%	0.104%
21	7.232	1833	1848	1864	rBV8	14184	28193	2.67%	0.244%
22	7.563	1939	1951	1962	rBV	89495	163343	15.46%	1.411%
23	7.894	2032	2054	2071	rBV	341372	634534	60.05%	5.481%
24	8.177	2129	2142	2153	rBV3	52050	94221	8.92%	0.814%
25	8.232	2155	2159	2172	rVB6	8516	14792	1.40%	0.128%
26	8.338	2182	2192	2208	rBV7	7047	15782	1.49%	0.136%
27	8.467	2223	2232	2244	rBV4	7043	11601	1.10%	0.100%
28	8.631	2271	2283	2324	rBV	460868	934068	88.39%	8.069%
29	9.412	2514	2526	2545	rBV	477863	837328	79.24%	7.233%
30	10.081	2723	2734	2752	rBV3	14630	26438	2.50%	0.228%
31	10.753	2920	2943	2959	rBV2	169845	361547	34.21%	3.123%
32	10.840	2959	2970	2979	rVV6	42115	80058	7.58%	0.692%
33	10.888	2979	2985	2990	rVV3	13710	22609	2.14%	0.195%
34	10.920	2990	2995	3006	rVB9	14041	21955	2.08%	0.190%
35	11.055	3027	3037	3048	rVB9	20072	36849	3.49%	0.318%
36	11.248	3079	3097	3106	rBV6	15397	30507	2.89%	0.264%

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

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 Title : TRACE VOA SFAM1.0

37	11.319	3109	3119	3132	rVV7	30190	71051	6.72%	0.614%
38	11.396	3132	3143	3154	rVB8	18162	34221	3.24%	0.296%
39	11.576	3189	3199	3209	rBV9	10099	17270	1.63%	0.149%
40	11.656	3209	3224	3230	rBV10	13193	29912	2.83%	0.258%
41	11.737	3230	3249	3260	rBV2	285187	518558	49.07%	4.480%
42	11.807	3260	3271	3293	rVB	525453	905440	85.69%	7.822%
43	11.904	3293	3301	3306	rBV4	25433	37047	3.51%	0.320%
44	11.939	3307	3312	3322	rVB3	35646	54248	5.13%	0.469%
45	12.007	3323	3333	3341	rBV6	28132	53160	5.03%	0.459%
46	12.055	3341	3348	3355	rBV3	44433	75603	7.15%	0.653%
47	12.187	3367	3389	3413	rVB2	429816	1056699	100.00%	9.128%
48	12.312	3417	3428	3438	rBV8	36012	69026	6.53%	0.596%
49	12.367	3438	3445	3454	rVB2	29266	42059	3.98%	0.363%
50	12.418	3455	3461	3469	rBV9	11811	17903	1.69%	0.155%
51	12.457	3470	3473	3484	rVB7	13626	17648	1.67%	0.152%
52	12.540	3484	3499	3504	rBV7	37328	77815	7.36%	0.672%
53	12.611	3515	3521	3525	rBV5	34501	47733	4.52%	0.412%
54	12.640	3526	3530	3540	rVB3	51077	69157	6.54%	0.597%
55	12.746	3556	3563	3569	rBV9	19749	33461	3.17%	0.289%
56	12.801	3574	3580	3588	rVB6	24865	39998	3.79%	0.346%
57	12.888	3599	3607	3616	rBV5	51838	85629	8.10%	0.740%
58	12.971	3623	3633	3646	rBV2	355381	581085	54.99%	5.020%
59	13.174	3689	3696	3705	rVB6	24657	35693	3.38%	0.308%
60	13.225	3707	3712	3722	rVB6	13468	23600	2.23%	0.204%
61	13.302	3726	3736	3748	rBV5	93029	169570	16.05%	1.465%
62	13.370	3749	3757	3764	rBV4	55320	79894	7.56%	0.690%
63	13.412	3764	3770	3777	rBV6	26415	38478	3.64%	0.332%
64	13.601	3821	3829	3840	rBV5	52159	85614	8.10%	0.740%
65	13.666	3841	3849	3851	rBV7	17472	22184	2.10%	0.192%
66	13.894	3911	3920	3933	rBV10	28627	60377	5.71%	0.522%
67	14.023	3946	3960	3971	rBV4	90082	164030	15.52%	1.417%
68	14.090	3975	3981	3997	rVB4	14640	33064	3.13%	0.286%
69	14.254	4025	4032	4036	rBV6	20039	30089	2.85%	0.260%
70	14.351	4057	4062	4073	rVB6	7721	13150	1.24%	0.114%
71	14.434	4073	4088	4094	rBV6	13802	30463	2.88%	0.263%
72	14.479	4096	4102	4120	rVB6	10129	25900	2.45%	0.224%
73	14.630	4135	4149	4161	rBV6	7790	21025	1.99%	0.182%
74	14.778	4188	4195	4204	rVB6	8557	14286	1.35%	0.123%
75	15.090	4286	4292	4303	rVB6	12517	20195	1.91%	0.174%

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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\SFAMUTR121123WMA.M
Title : TRACE VOA SFAM1.0

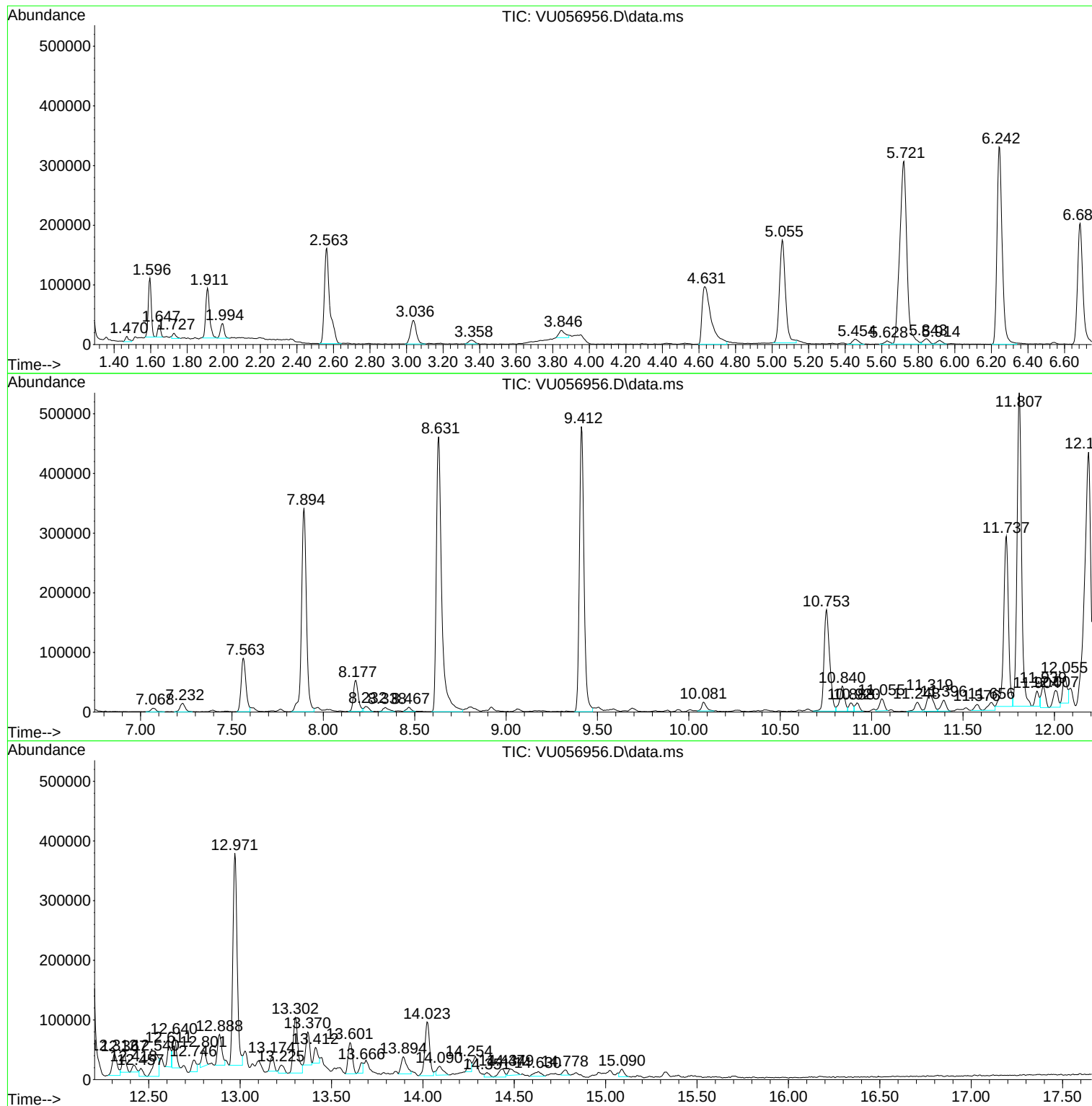
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

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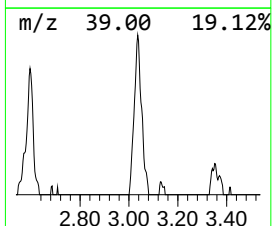
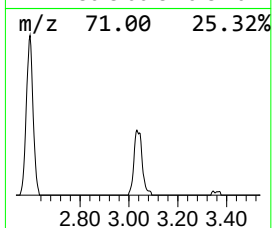
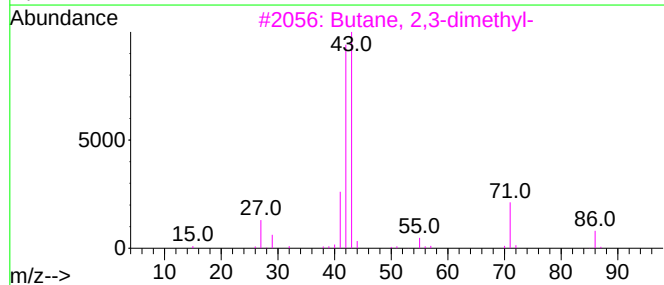
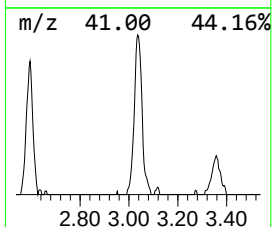
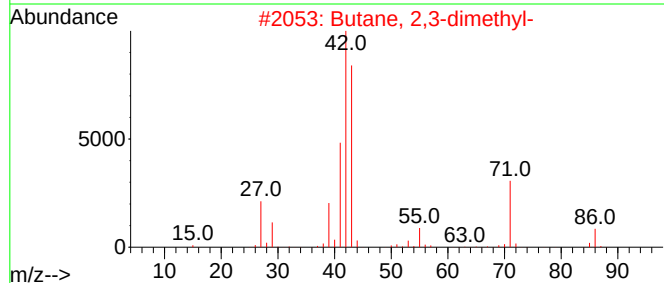
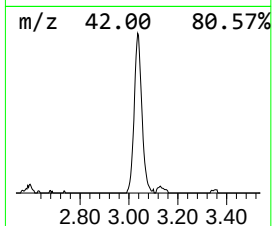
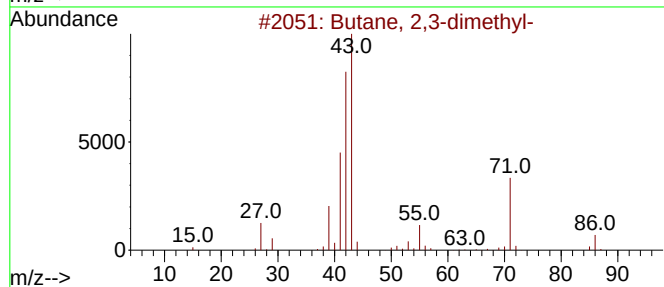
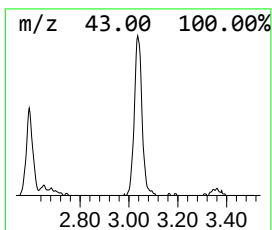
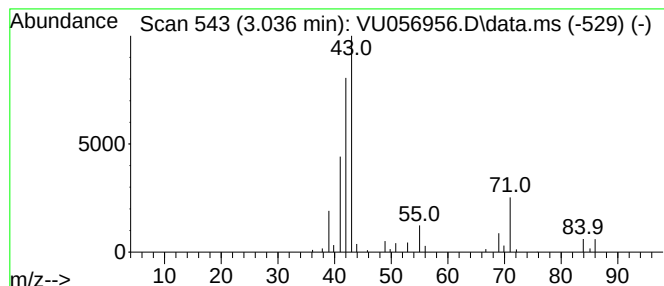
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.036	0.66 ug/L	85828	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64



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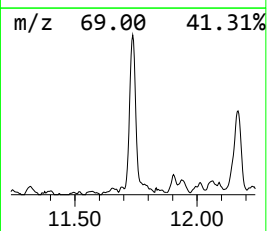
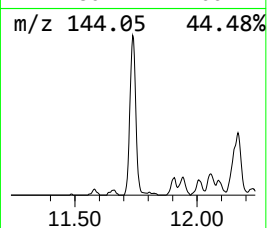
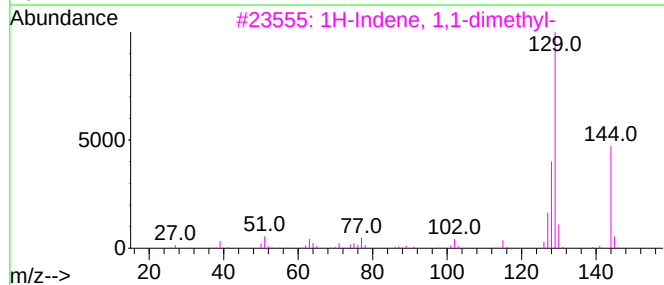
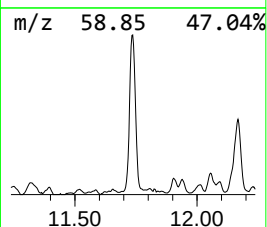
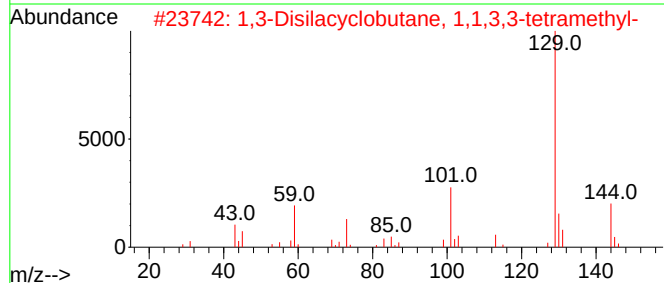
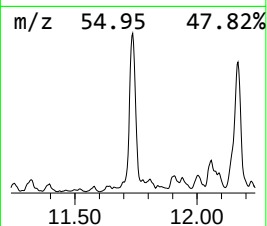
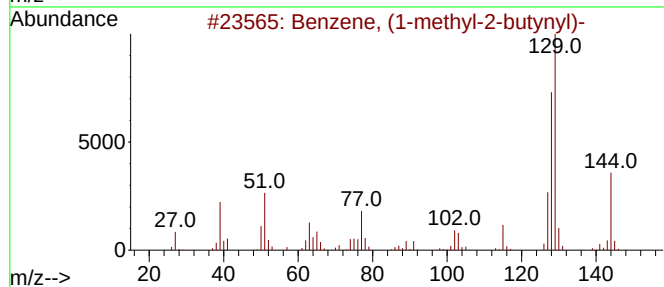
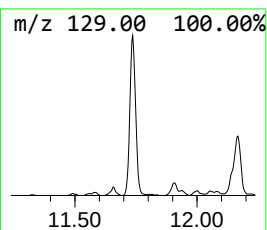
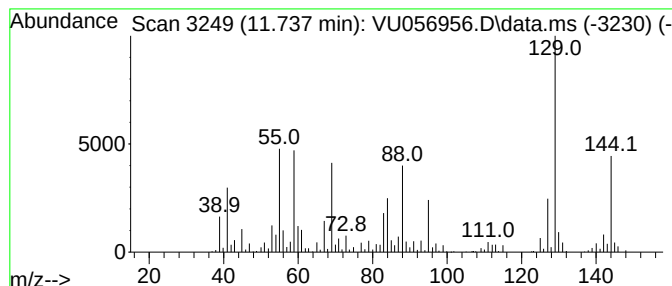
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.737	2.86 ug/L	518558	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-butynyl)-	144	C11H12	087712-69-4	43
2			1,3-Disilacyclobutane, 1,1,3,3-t...	144	C6H16Si2	001627-98-1	43
3			1H-Indene, 1,1-dimethyl-	144	C11H12	018636-55-0	38
4			1-Methoxy-1-methyl-1-silacyclohe...	144	C7H16OSi	020089-28-5	37
5			1H-Indene, 2,3-dimethyl-	144	C11H12	004773-82-4	35



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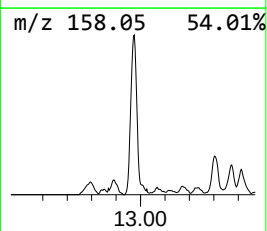
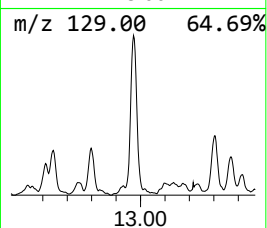
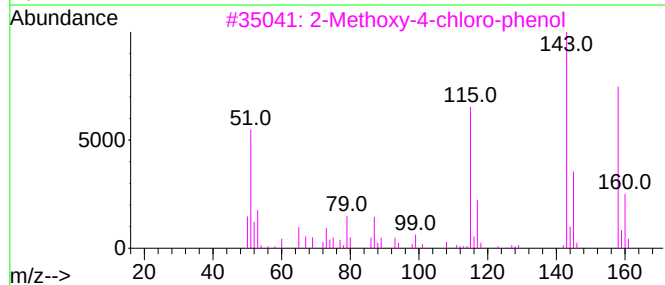
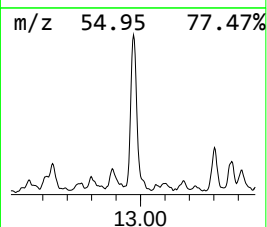
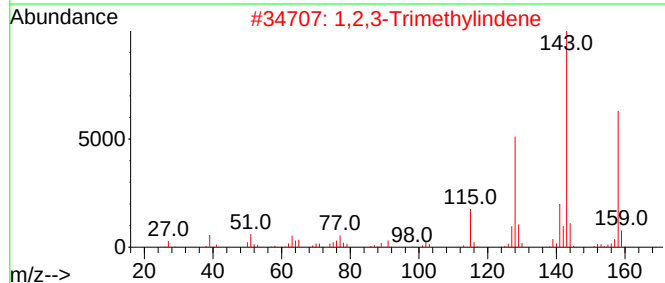
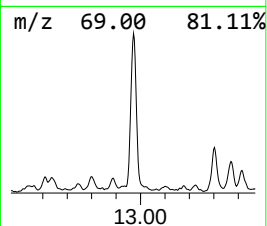
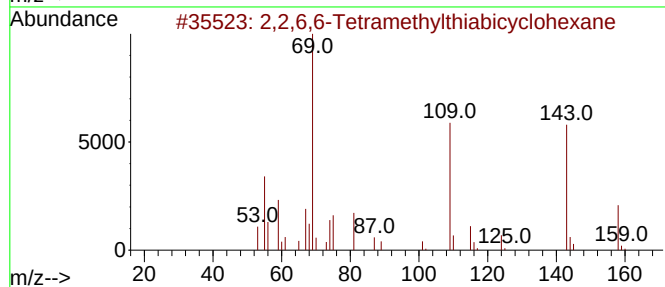
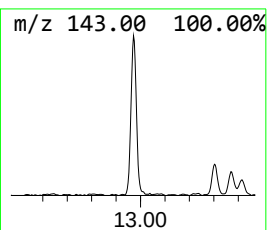
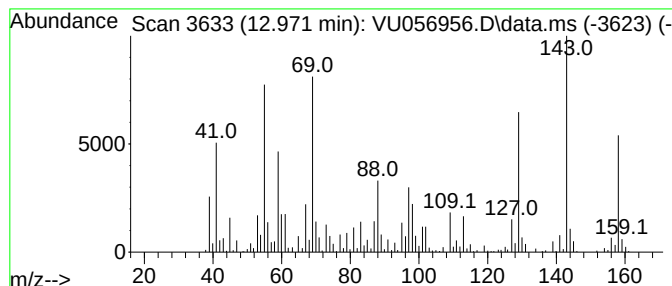
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2,2,6,6-Tetramethylthiacyclo... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.971	3.21 ug/L	581085	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,6,6-Tetramethylthiacyclohe...	158	C9H18S	078050-22-3	58		
2	1,2,3-Trimethylindene	158	C12H14	004773-83-5	25		
3	2-Methoxy-4-chloro-phenol	158	C7H7ClO2	016766-30-6	25		
4	3-Methyl-3-hexene	98	C7H14	003404-65-7	25		
5	1H-Indene, 1,1,3-trimethyl-	158	C12H14	002177-45-9	25		



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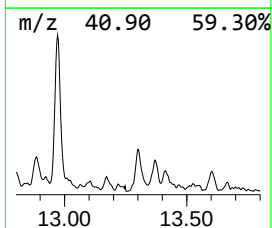
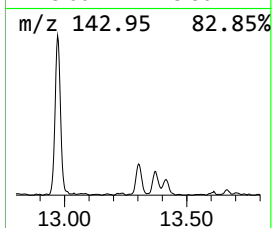
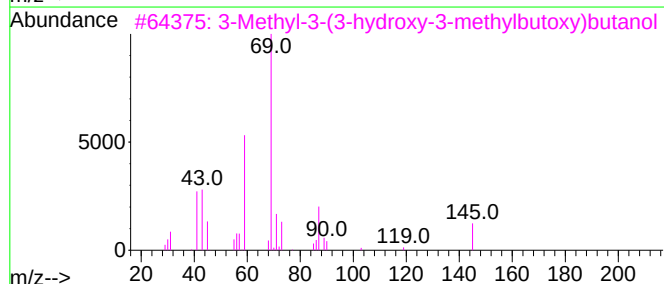
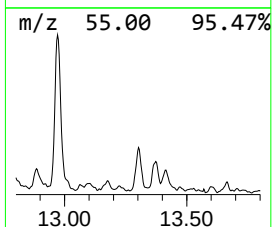
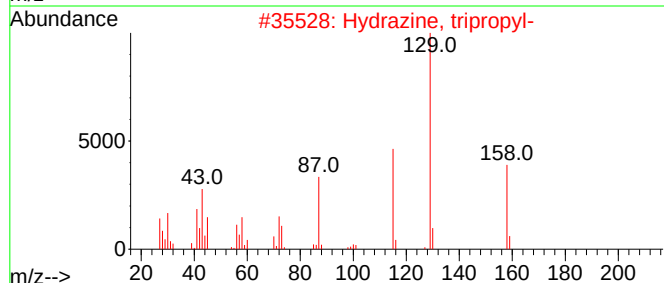
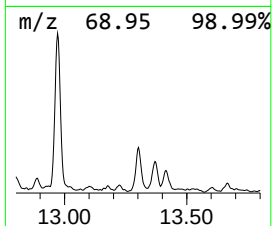
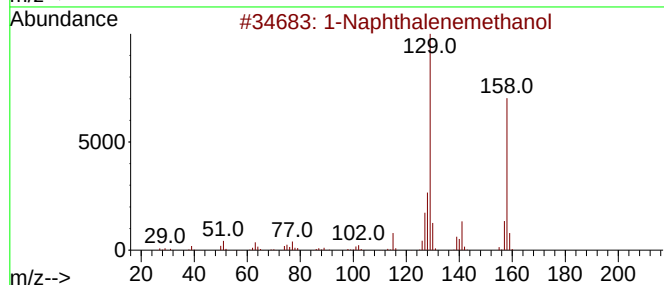
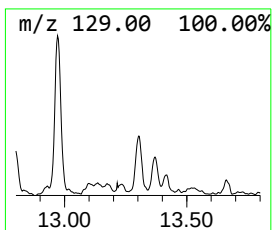
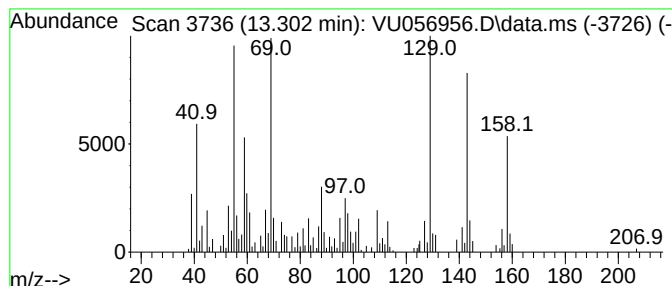
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.302	0.94 ug/L	169570	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Naphthalenemethanol	158	C11H10O	004780-79-4	18
2			Hydrazine, tripropyl-	158	C9H22N2	067398-42-9	14
3			3-Methyl-3-(3-hydroxy-3-methylbu...	190	C10H22O3	1000432-16-8	14
4			4H-1,2,4-Triazole, 4-methyl-3-(m...	129	C4H7N3S	021094-61-1	11
5			Goitrin	129	C5H7NO5	000500-12-9	11



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121623\
Data File : VU056956.D
Acq On : 17 Dec 2023 05:06
Operator : MD/SY
Sample : 05811-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F7B40

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	3.036	0.7	ug/L	85828	1	6.245	653606	5.0
unknown-01	11.737	2.9	ug/L	518558	3	11.807	905440	5.0
2,2,6,6-Tetrame...	12.971	3.2	ug/L	581085	3	11.807	905440	5.0
unknown-02	13.302	0.9	ug/L	169570	3	11.807	905440	5.0