

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122023\
 Data File : VU057122.D
 Acq On : 21 Dec 2023 04:39
 Operator : MD/SY
 Sample : 05892-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 47 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F7B17

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: VU057122.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	15	21	23	rBV2	17556	18109	2.94%	0.280%
2	1.486	58	61	68	rVB2	13068	11917	1.93%	0.184%
3	1.596	85	95	104	rBV	86049	107044	17.37%	1.653%
4	1.911	185	193	206	rVB	65289	89170	14.47%	1.377%
5	1.991	210	218	227	rVB	55429	75460	12.24%	1.165%
6	2.563	384	396	416	rVB2	143822	259515	42.11%	4.007%
7	2.789	457	466	478	rBV2	5109	8897	1.44%	0.137%
8	3.033	528	542	554	rBV7	6780	15045	2.44%	0.232%
9	4.637	1026	1041	1082	rBV2	43805	165013	26.78%	2.548%
10	5.055	1154	1171	1197	rBV2	134904	304366	49.39%	4.700%
11	5.718	1357	1377	1412	rVB3	236530	616254	100.00%	9.516%
12	6.242	1527	1540	1566	rBV	224452	436457	70.82%	6.739%
13	6.682	1663	1677	1707	rBV	149437	296761	48.16%	4.582%
14	7.158	1810	1825	1840	rBV3	8977	18279	2.97%	0.282%
15	7.393	1885	1898	1909	rBV6	5781	10077	1.64%	0.156%
16	7.560	1936	1950	1965	rBV2	63272	113601	18.43%	1.754%
17	7.891	2035	2053	2069	rBV	268268	482346	78.27%	7.448%
18	7.965	2069	2076	2086	rVB3	9157	16716	2.71%	0.258%
19	8.174	2129	2141	2155	rBV2	39645	70068	11.37%	1.082%
20	8.332	2181	2190	2198	rBV5	10626	17576	2.85%	0.271%
21	8.406	2203	2213	2222	rVB6	6876	13214	2.14%	0.204%
22	8.631	2270	2283	2314	rBV2	228846	466324	75.67%	7.201%
23	9.258	2470	2478	2487	rBV7	4776	7966	1.29%	0.123%
24	9.412	2512	2526	2547	rBV	334281	583062	94.61%	9.003%
25	9.570	2568	2575	2585	rBV5	10592	20648	3.35%	0.319%
26	9.939	2683	2690	2699	rBV4	6635	9051	1.47%	0.140%
27	10.007	2699	2711	2718	rBV7	6149	9537	1.55%	0.147%
28	10.078	2721	2733	2747	rVB2	28709	51132	8.30%	0.790%
29	10.341	2807	2815	2827	rBV8	9065	16452	2.67%	0.254%
30	10.750	2927	2942	2957	rBV	108144	210403	34.14%	3.249%
31	10.840	2964	2970	2980	rVB6	13308	19811	3.21%	0.306%
32	11.055	3029	3037	3046	rVV9	7368	11592	1.88%	0.179%
33	11.110	3046	3054	3064	rVB3	6176	10714	1.74%	0.165%
34	11.238	3085	3094	3106	rVB3	7704	17154	2.78%	0.265%
35	11.319	3108	3119	3130	rBV3	12753	26136	4.24%	0.404%
36	11.393	3132	3142	3156	rVB10	10995	20658	3.35%	0.319%

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37	11.576	3190	3199	3209	rBV10	5070	8663	1.41%	0.134%
38	11.653	3209	3223	3227	rBV10	6877	13090	2.12%	0.202%
39	11.695	3228	3236	3239	rVV6	9280	13907	2.26%	0.215%
40	11.737	3240	3249	3259	rVB2	70160	117060	19.00%	1.808%
41	11.807	3259	3271	3292	rVB	341531	562815	91.33%	8.691%
42	11.939	3306	3312	3319	rVB8	6226	7583	1.23%	0.117%
43	12.000	3320	3331	3340	rVB8	9022	21984	3.57%	0.339%
44	12.052	3340	3347	3348	rBV5	12750	10543	1.71%	0.163%
45	12.187	3367	3389	3416	rVB	289521	585166	94.96%	9.036%
46	12.315	3418	3429	3438	rBV7	14885	29071	4.72%	0.449%
47	12.364	3438	3444	3454	rVB4	9487	13339	2.16%	0.206%
48	12.541	3492	3499	3503	rBV4	6446	8890	1.44%	0.137%
49	12.611	3514	3521	3526	rBV6	11825	17510	2.84%	0.270%
50	12.640	3526	3530	3537	rVB6	14106	18147	2.94%	0.280%
51	12.750	3556	3564	3572	rBV6	5898	9731	1.58%	0.150%
52	12.798	3574	3579	3588	rBV10	4349	6267	1.02%	0.097%
53	12.885	3596	3606	3615	rBV10	10399	18581	3.02%	0.287%
54	12.971	3623	3633	3658	rVB4	68149	128107	20.79%	1.978%
55	13.171	3688	3695	3705	rBV10	5668	10575	1.72%	0.163%
56	13.303	3724	3736	3747	rBV8	15675	28704	4.66%	0.443%
57	13.370	3750	3757	3765	rVV6	12193	18812	3.05%	0.290%
58	13.415	3765	3771	3773	rVV6	6272	7558	1.23%	0.117%
59	13.444	3777	3780	3786	rVB7	7207	7266	1.18%	0.112%
60	13.602	3822	3829	3842	rBV10	11335	20037	3.25%	0.309%
61	13.891	3910	3919	3931	rVV10	6404	11626	1.89%	0.180%
62	14.023	3952	3960	3971	rVB6	16492	25556	4.15%	0.395%
63	14.187	4001	4011	4023	rBV5	20408	31367	5.09%	0.484%
64	14.258	4023	4033	4038	rBV5	4897	9492	1.54%	0.147%
65	15.682	4467	4476	4487	rBV9	11676	18760	3.04%	0.290%
66	15.939	4547	4556	4565	rBV7	12087	18705	3.04%	0.289%
67	16.878	4838	4848	4858	rBV2	33948	50709	8.23%	0.783%

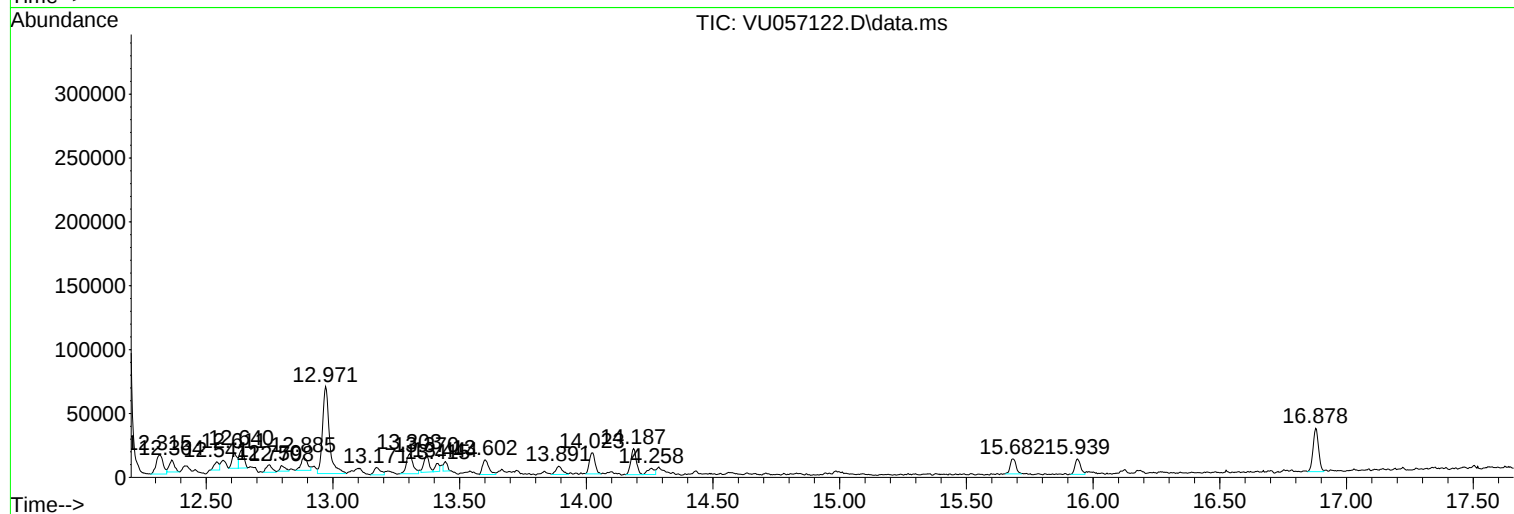
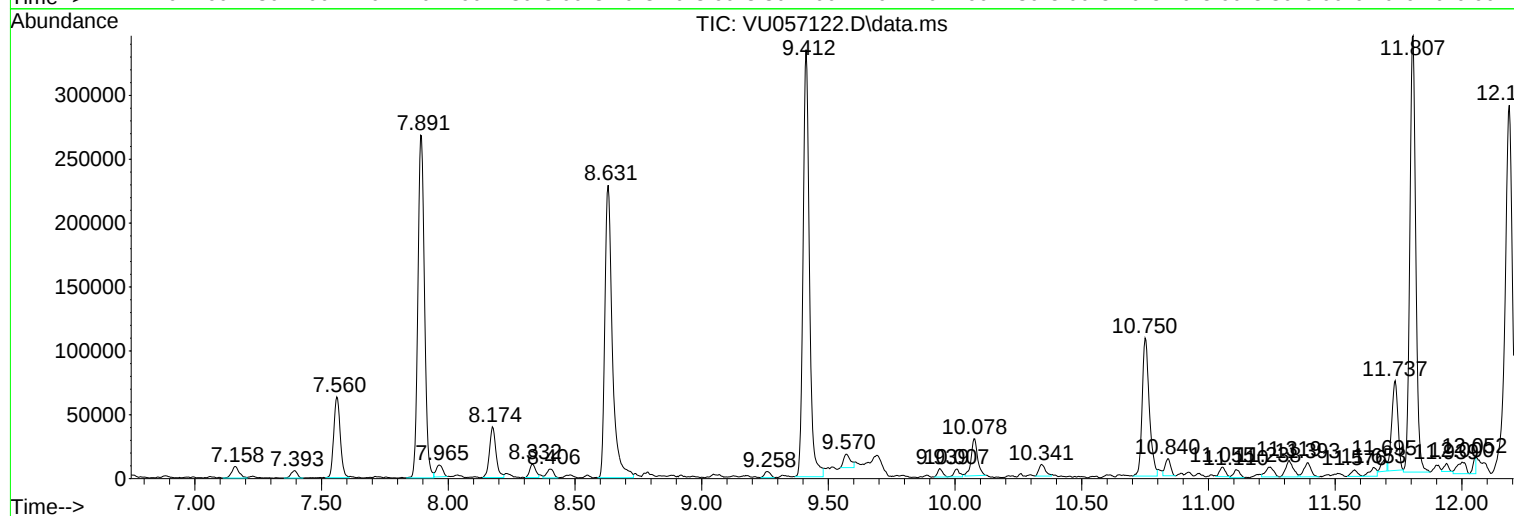
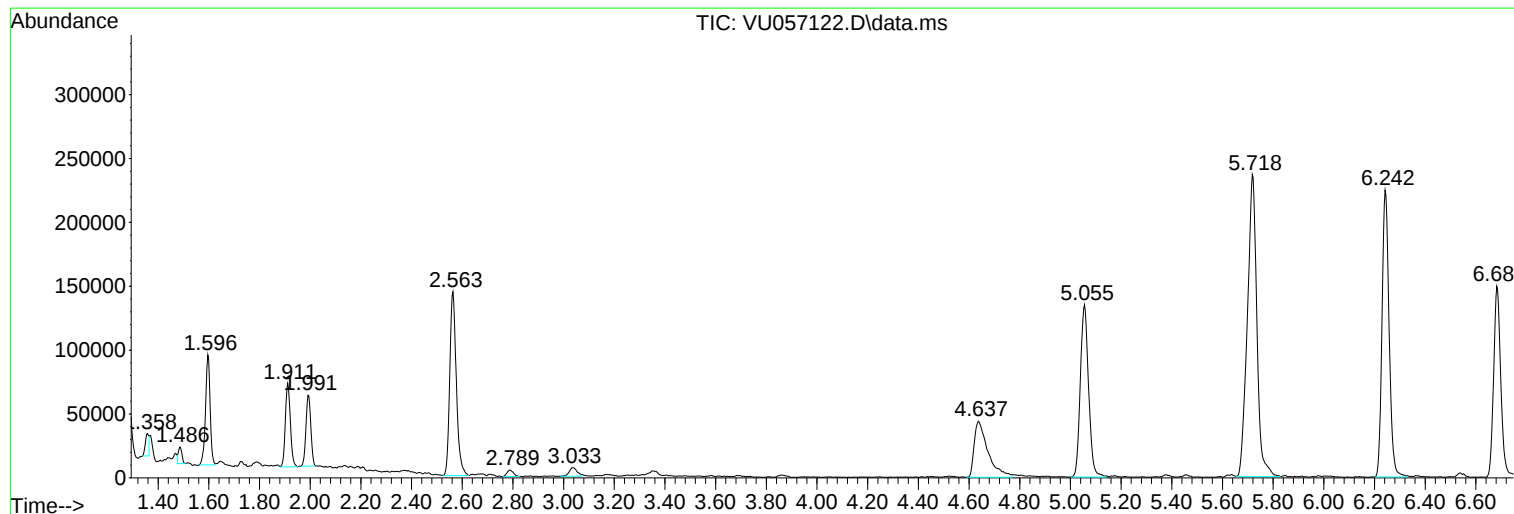
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 47 Sample Multiplier: 1

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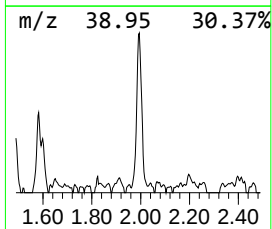
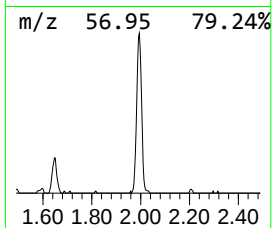
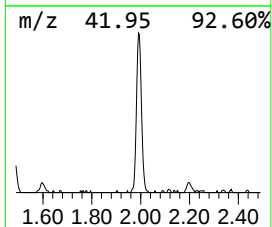
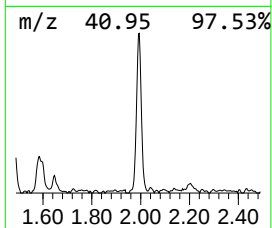
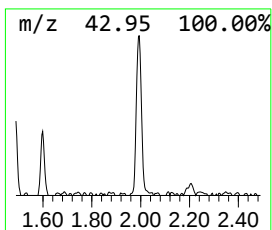
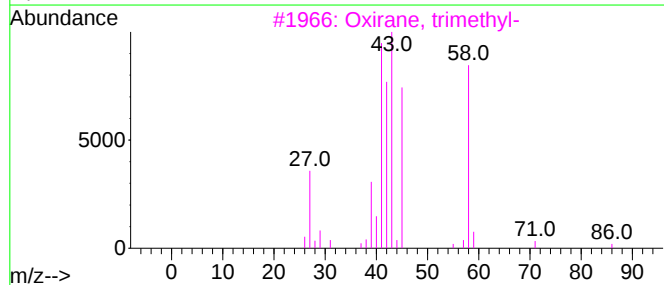
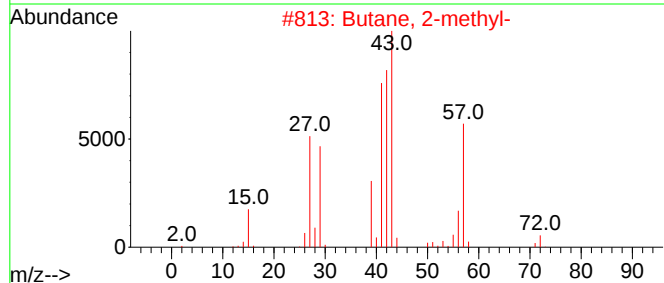
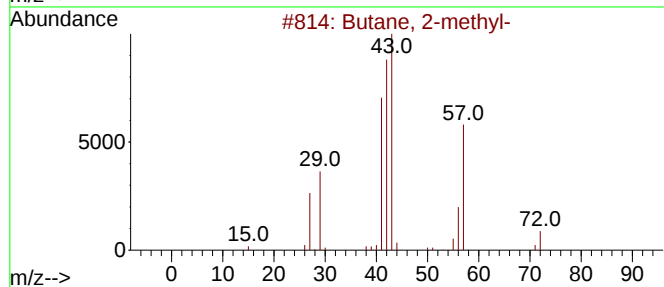
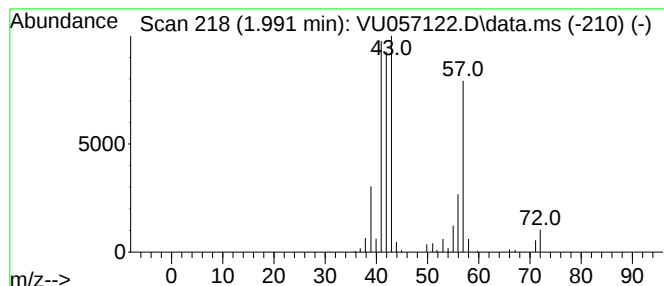
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.991	0.86 ug/L	75460	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	86
2	Butane, 2-methyl-			72	C5H12	000078-78-4	80
3	Oxirane, trimethyl-			86	C5H10O	005076-19-7	33
4	Pentane			72	C5H12	000109-66-0	28
5	Isobutylene epoxide			72	C4H8O	000558-30-5	28



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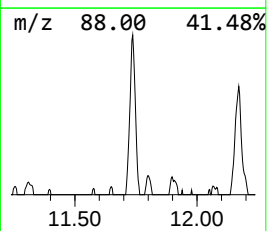
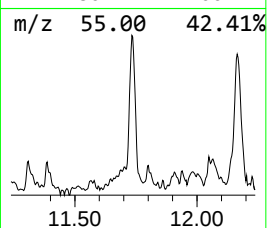
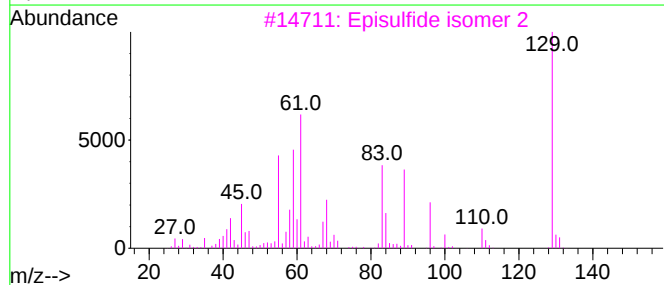
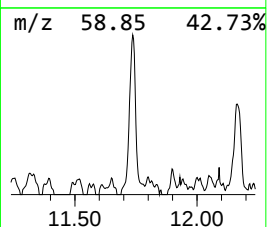
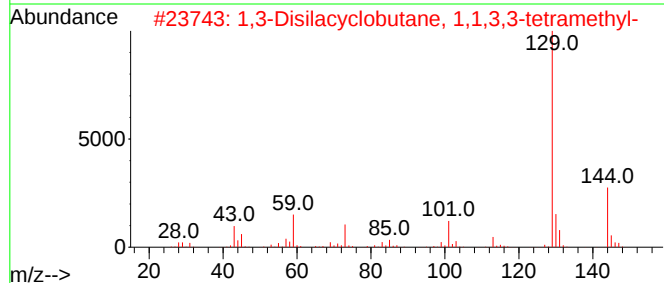
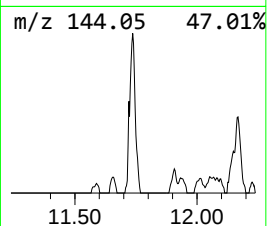
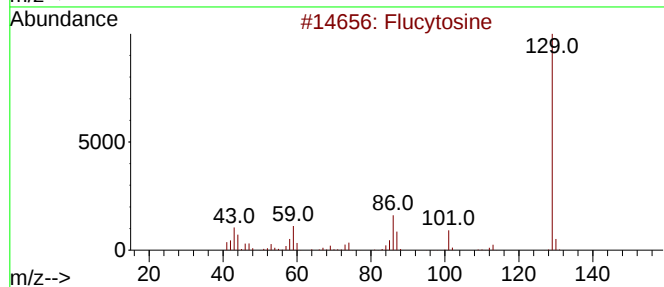
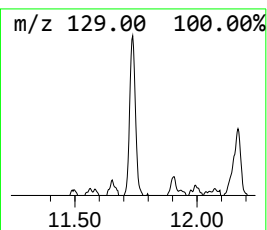
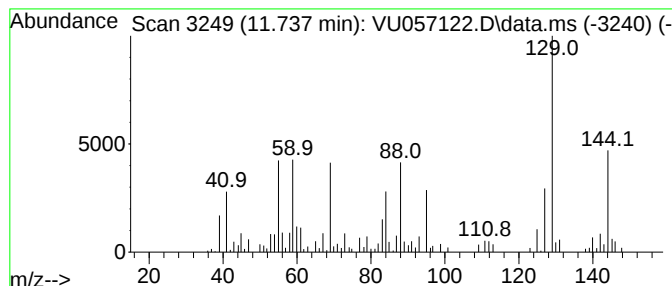
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.737	1.04 ug/L	117060	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Flucytosine	129	C4H4FN3O	002022-85-7	27
2			1,3-Disilacyclobutane, 1,1,3,3-t...	144	C6H16Si2	001627-98-1	25
3			Episulfide isomer 2	129	C5H7NOS	030381-35-2	25
4			1H-Indene, 1,1-dimethyl-	144	C11H12	018636-55-0	25
5			1H-Cyclopropa[b]naphthalene, 1a,...	144	C11H12	006571-72-8	17



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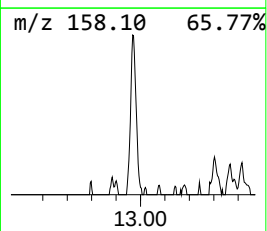
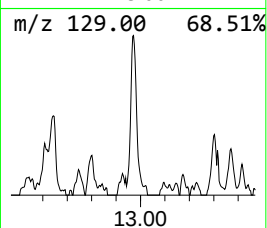
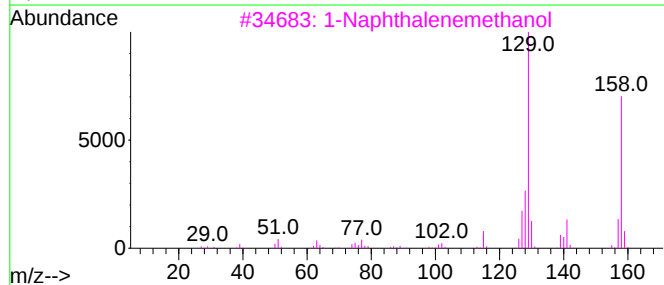
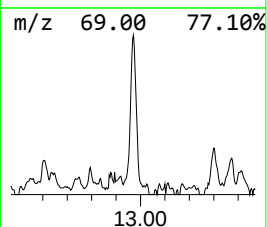
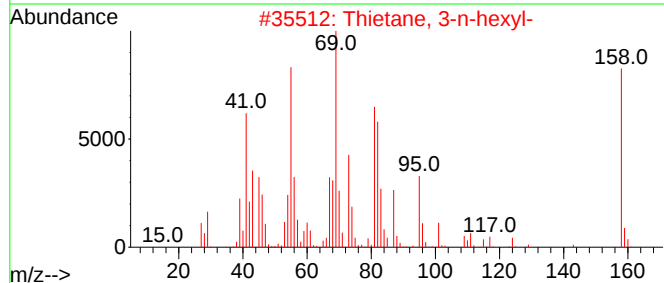
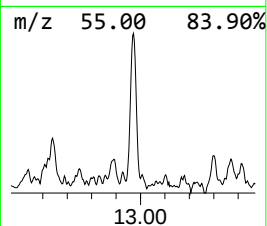
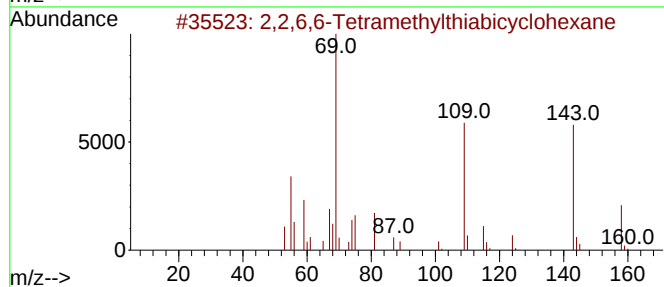
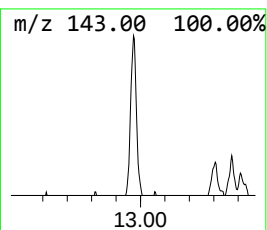
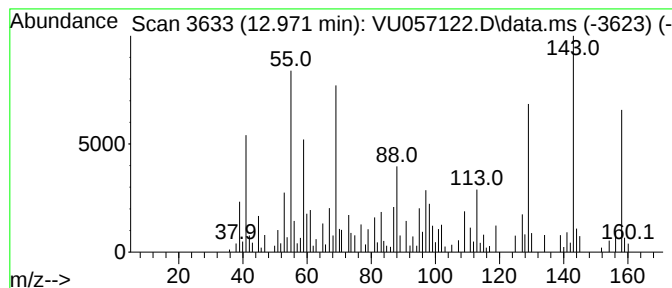
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.971	1.14 ug/L	128107	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,6,6-Tetramethylthiabicyclohe...	158	C9H18S	078050-22-3	49		
2	Thietane, 3-n-hexyl-	158	C9H18S	1000491-56-1	35		
3	1-Naphthalenemethanol	158	C11H10O	004780-79-4	15		
4	2-Pentenal, 2-methyl-	98	C6H10O	000623-36-9	11		
5	3-Hexene, 3-methyl-, (E)-	98	C7H14	003899-36-3	11		



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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
(DEL) Alkane: S...	1.991	0.9	ug/L	75460	1	6.242	436457	5.0
unknown-01	11.737	1.0	ug/L	117060	3	11.807	562815	5.0
unknown-02	12.971	1.1	ug/L	128107	3	11.807	562815	5.0