

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV063022\
 Data File : VV026600.D
 Acq On : 30 Jun 2022 12:18
 Operator : SY/MD
 Sample : N3534-05
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 A0AH0

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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\SFAMVLM062922WMA.M

Title : VOC Analysis

Signal : TIC: VV026600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.146	26	33	52	rBV	203182	190568	2.30%	0.489%
2	1.227	52	58	62	rBV	57229	55929	0.68%	0.143%
3	1.256	62	67	80	rVV	165392	195415	2.36%	0.501%
4	1.323	81	88	132	rVB2	523968	640148	7.74%	1.642%
5	1.558	147	161	200	rBV2	639720	1497958	18.10%	3.842%
6	1.764	217	225	243	rVB	498280	647972	7.83%	1.662%
7	2.124	325	337	347	rBV3	1074345	1781076	21.53%	4.568%
8	2.191	347	358	425	rVB	3988861	8274120	100.00%	21.220%
9	2.516	448	459	481	rVB	378315	625141	7.56%	1.603%
10	2.677	507	509	513	rVB3	662	364	0.00%	0.001%
11	2.770	526	538	563	rVV	175135	305972	3.70%	0.785%
12	2.989	603	606	609	rVB2	384	281	0.00%	0.001%
13	3.050	619	625	628	rVB2	559	417	0.01%	0.001%
14	3.201	655	672	700	rBV	402937	851674	10.29%	2.184%
15	3.452	745	750	752	rBV2	340	261	0.00%	0.001%
16	3.584	786	791	797	rVB3	439	599	0.01%	0.002%
17	3.767	845	848	851	rBV	342	249	0.00%	0.001%
18	3.863	874	878	881	rBV3	343	319	0.00%	0.001%
19	3.921	881	896	929	rBV3	326732	915845	11.07%	2.349%
20	4.256	986	1000	1018	rBV2	213482	529831	6.40%	1.359%
21	4.375	1019	1037	1077	rVB4	472104	1600269	19.34%	4.104%
22	4.616	1096	1112	1133	rVB2	143665	355344	4.29%	0.911%
23	4.757	1153	1156	1159	rVB2	430	279	0.00%	0.001%
24	4.834	1161	1180	1208	rBV	371131	882628	10.67%	2.264%
25	5.053	1230	1248	1256	rBV2	652603	1600748	19.35%	4.105%
26	5.452	1361	1372	1374	rBV3	2771	3329	0.04%	0.009%
27	5.538	1395	1399	1403	rBV4	347	344	0.00%	0.001%
28	5.577	1408	1411	1412	rBV	626	323	0.00%	0.001%
29	5.619	1412	1424	1453	rBV	470878	945735	11.43%	2.425%
30	5.915	1503	1516	1551	rVV	840915	1650941	19.95%	4.234%
31	6.072	1552	1565	1585	rVV	368578	749065	9.05%	1.921%
32	6.175	1585	1597	1633	rVB	349138	700490	8.47%	1.796%
33	6.320	1638	1642	1646	rBV5	1368	1387	0.02%	0.004%
34	6.365	1654	1656	1659	rVB3	529	255	0.00%	0.001%
35	6.513	1687	1702	1722	rBV	130475	251334	3.04%	0.645%
36	6.651	1731	1745	1766	rBV4	11301	31291	0.38%	0.080%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062922WMA.M
 Title : VOC Analysis

37	6.825	1795	1799	1803	rBV4	601	598	0.01%	0.002%
38	6.876	1811	1815	1816	rBV3	333	273	0.00%	0.001%
39	6.989	1838	1850	1856	rBV	182563	315231	3.81%	0.808%
40	7.027	1857	1862	1894	rVV	192710	352701	4.26%	0.905%
41	7.162	1896	1904	1928	rVB2	22465	52227	0.63%	0.134%
42	7.317	1939	1952	1970	rBV	748460	1291551	15.61%	3.312%
43	7.622	2037	2047	2049	rBV	142490	171971	2.08%	0.441%
44	7.651	2051	2056	2083	rVB	325828	541968	6.55%	1.390%
45	7.837	2103	2114	2142	rVB	284606	496056	6.00%	1.272%
46	7.972	2143	2156	2178	rBV	945617	1568345	18.95%	4.022%
47	8.091	2183	2193	2229	rVV	333719	660321	7.98%	1.693%
48	8.246	2229	2241	2263	rVB	239297	403084	4.87%	1.034%
49	8.352	2263	2274	2293	rBV	163591	280513	3.39%	0.719%
50	8.519	2325	2326	2332	rVB2	512	398	0.00%	0.001%
51	8.548	2332	2335	2338	rBV3	625	467	0.01%	0.001%
52	8.587	2344	2347	2350	rVB2	636	365	0.00%	0.001%
53	8.615	2353	2356	2357	rBV3	534	324	0.00%	0.001%
54	8.667	2369	2372	2378	rVB3	568	475	0.01%	0.001%
55	8.850	2414	2429	2455	rBV	719118	1176976	14.22%	3.018%
56	8.972	2455	2467	2494	rVB	663372	1100343	13.30%	2.822%
57	9.066	2494	2496	2504	rVB6	1006	746	0.01%	0.002%
58	9.104	2504	2508	2510	rBV2	684	467	0.01%	0.001%
59	9.133	2514	2517	2518	rBV3	983	526	0.01%	0.001%
60	9.384	2590	2595	2603	rVB3	382	457	0.01%	0.001%
61	9.496	2628	2630	2639	rVB4	648	673	0.01%	0.002%
62	9.551	2640	2647	2653	rBV	1025	1182	0.01%	0.003%
63	9.590	2655	2659	2662	rVB3	538	466	0.01%	0.001%
64	9.728	2691	2702	2722	rBV	180953	305378	3.69%	0.783%
65	9.863	2741	2744	2752	rVB2	479	562	0.01%	0.001%
66	9.927	2752	2764	2766	rBV4	687	1014	0.01%	0.003%
67	10.123	2819	2825	2837	rVB6	2084	3379	0.04%	0.009%
68	10.217	2837	2854	2858	rBV	543614	899417	10.87%	2.307%
69	10.313	2882	2884	2887	rVB3	589	247	0.00%	0.001%
70	10.541	2948	2955	2962	rBV3	1937	2740	0.03%	0.007%
71	10.567	2962	2963	2965	rBV	713	393	0.00%	0.001%
72	10.738	3009	3016	3027	rVB3	3530	4990	0.06%	0.013%
73	10.869	3047	3057	3060	rBV5	3355	4672	0.06%	0.012%
74	10.914	3060	3071	3095	rVB	999952	1445157	17.47%	3.706%
75	11.140	3137	3141	3149	rBV3	1040	1375	0.02%	0.004%
76	11.194	3149	3158	3163	rVB7	2035	3057	0.04%	0.008%

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 Title : VOC Analysis

77	11.246	3163	3174	3198	rBV	793951	1213084	14.66%	3.111%
78	11.381	3212	3216	3217	rBV3	818	614	0.01%	0.002%
79	11.622	3279	3291	3310	rBV	744098	1157872	13.99%	2.969%
80	11.779	3339	3340	3346	rVB3	613	577	0.01%	0.001%
81	11.811	3346	3350	3352	rBV2	368	262	0.00%	0.001%
82	11.853	3360	3363	3367	rVB2	429	276	0.00%	0.001%
83	11.882	3368	3372	3373	rBV2	434	267	0.00%	0.001%
84	12.091	3435	3437	3445	rVB4	360	333	0.00%	0.001%
85	12.426	3530	3541	3562	rVB	140642	222067	2.68%	0.570%
86	12.647	3603	3610	3613	rBV5	1784	1772	0.02%	0.005%
87	12.808	3658	3660	3664	rBV	408	305	0.00%	0.001%
88	13.191	3773	3779	3781	rBV3	330	411	0.00%	0.001%
89	13.265	3796	3802	3811	rVB3	2173	2991	0.04%	0.008%
90	13.348	3822	3828	3830	rBV2	346	365	0.00%	0.001%
91	13.438	3851	3856	3859	rBV3	482	408	0.00%	0.001%
92	13.506	3869	3877	3888	rBV3	3841	5573	0.07%	0.014%
93	13.622	3908	3913	3916	rVB	414	352	0.00%	0.001%
94	13.692	3926	3935	3936	rBV2	462	542	0.01%	0.001%
95	13.747	3944	3952	3959	rBV6	2098	3250	0.04%	0.008%
96	13.860	3983	3987	3991	rBV4	449	401	0.00%	0.001%
97	13.895	3996	3998	4002	rVB3	518	350	0.00%	0.001%
98	14.310	4124	4127	4130	rBV2	351	276	0.00%	0.001%
99	14.541	4196	4199	4203	rBV2	417	390	0.00%	0.001%
100	15.171	4392	4395	4399	rBV2	702	546	0.01%	0.001%

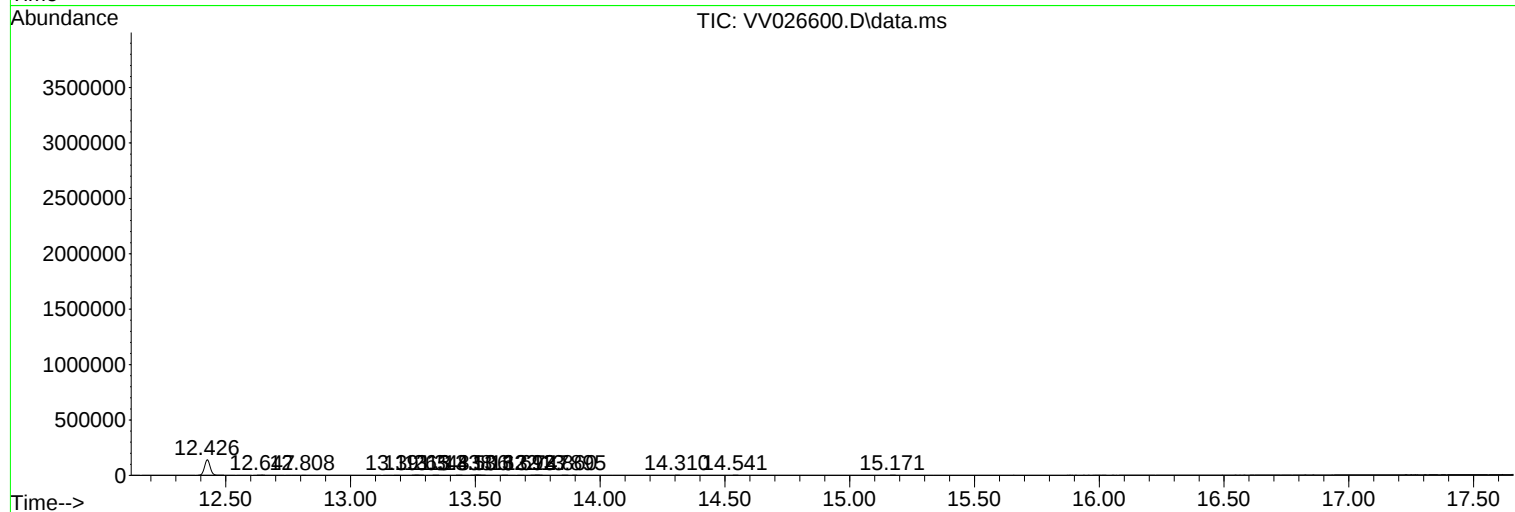
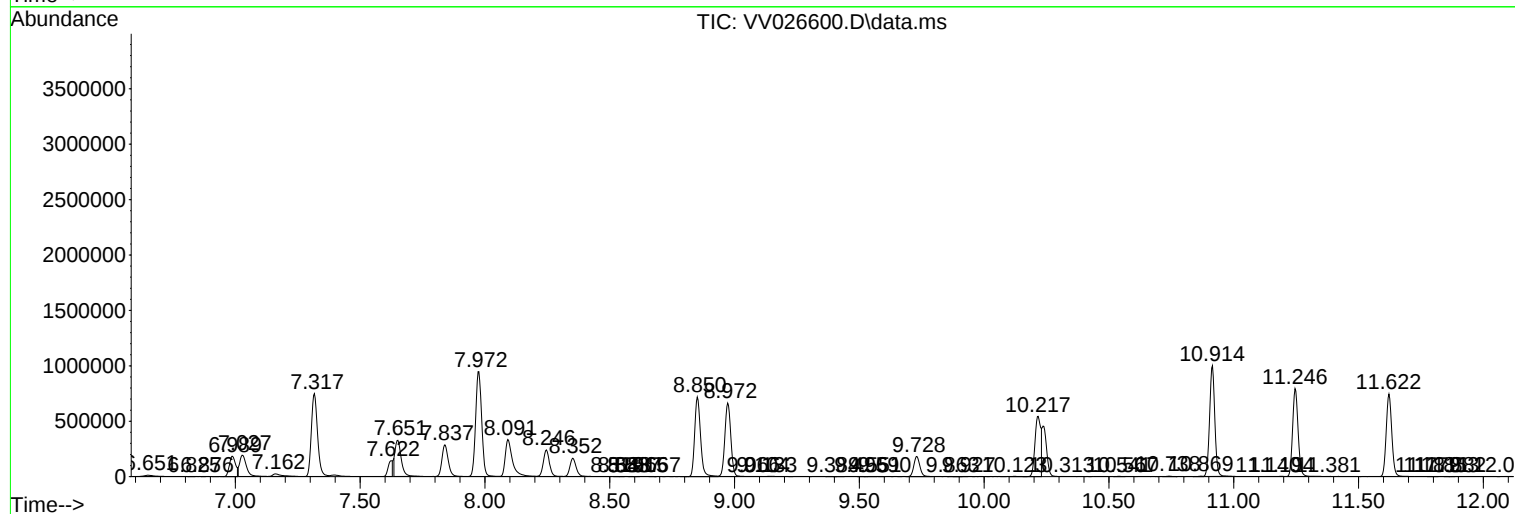
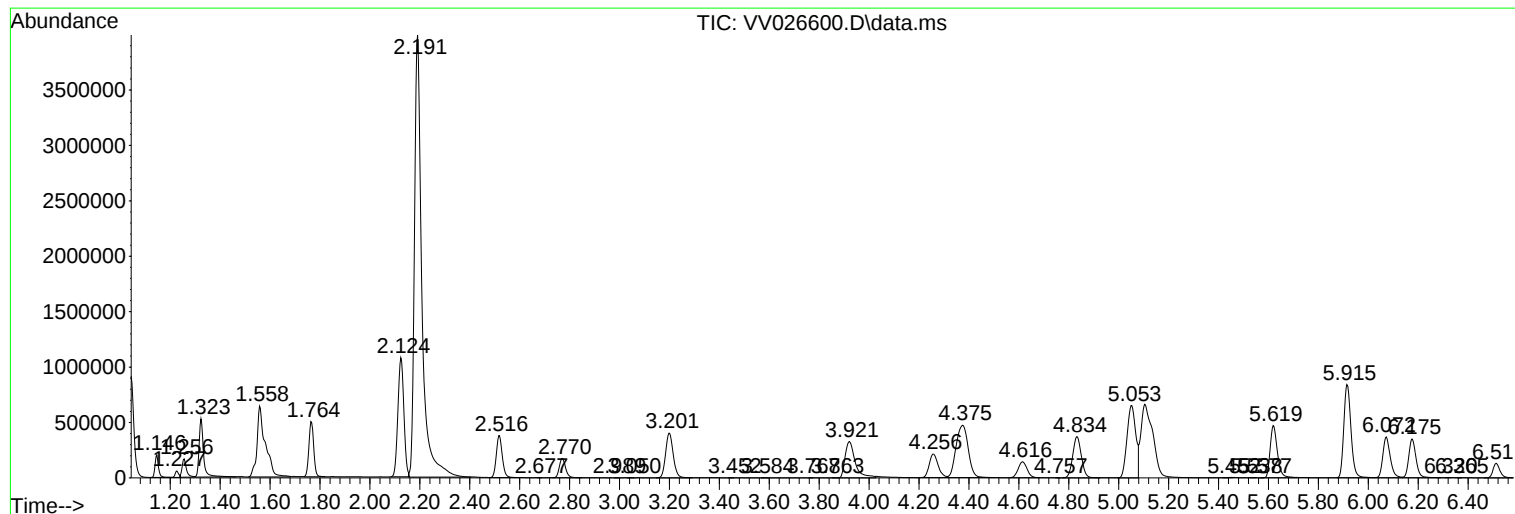
Sum of corrected areas: 38992270

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062922WMA.M
Quant Title : VOC Analysis

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



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A0AH0

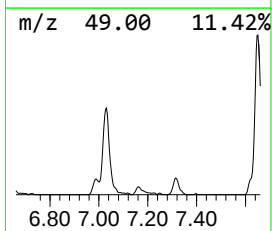
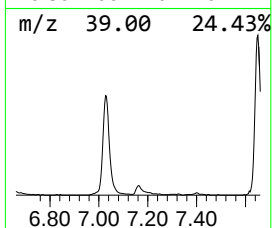
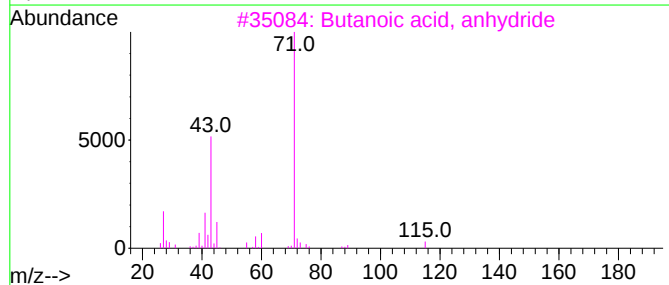
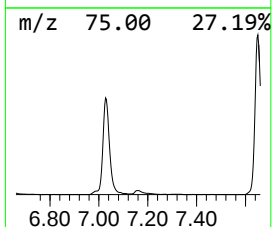
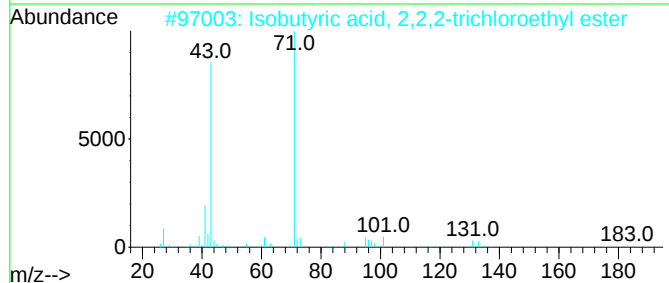
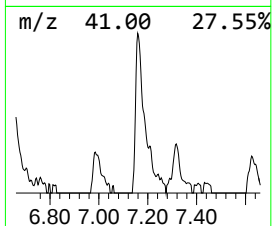
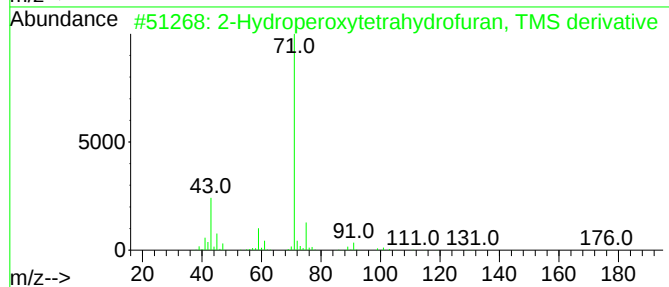
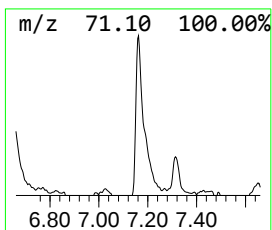
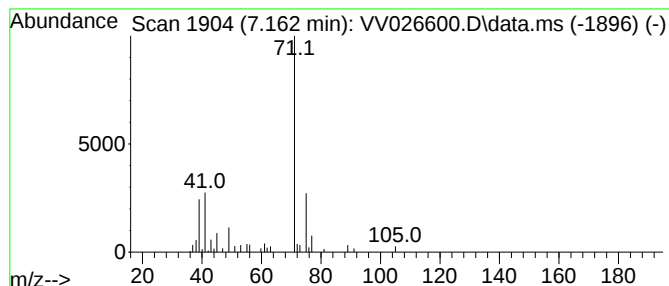
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062922WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 2-Hydroperoxytetrahydrofura... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.162	2.76 ug/L	52227	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	64
2			Isobutyric acid, 2,2,2-trichloro...	218	C6H9Cl3O2	1000354-63-4	36
3			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	9
4			Butanoyl chloride	106	C4H7ClO	000141-75-3	9
5			1,5-Heptadiene-3,4-diol, 2-methyl-	142	C8H14O2	022726-05-2	9



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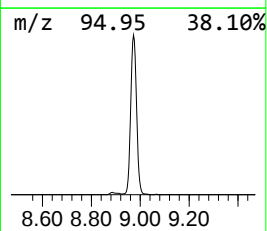
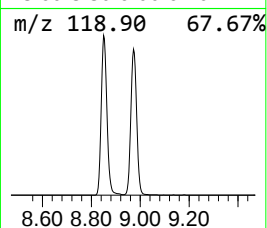
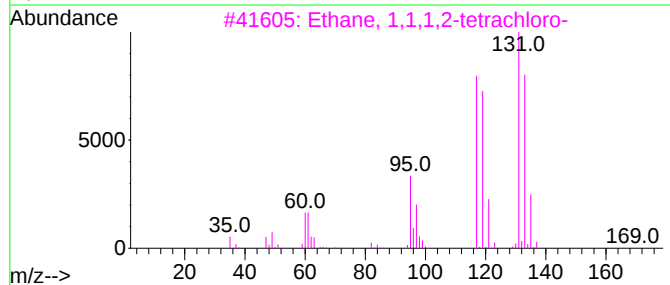
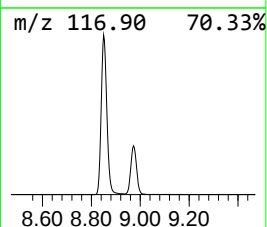
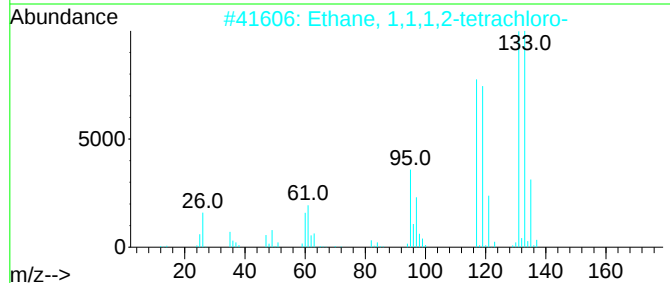
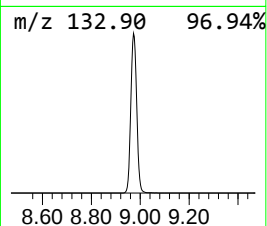
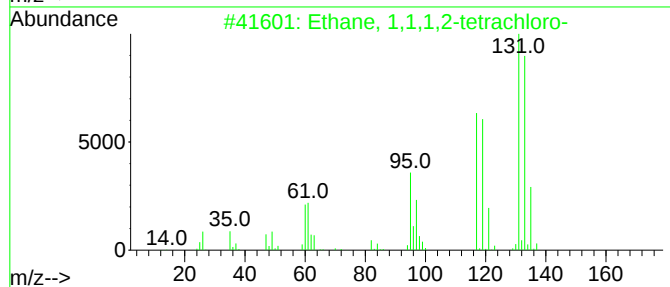
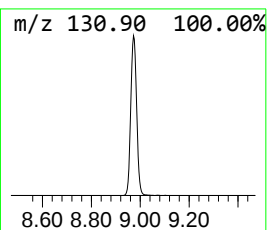
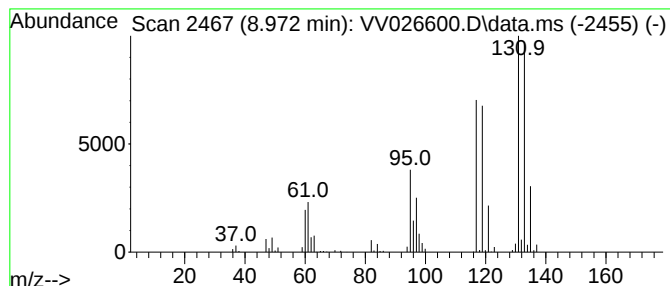
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM062922WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Ethane, 1,1,1,2-tetrachloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.972	46.74 ug/L	1100340	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
2			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	91
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	72
5			Carbon Tetrachloride	152	CCl4	000056-23-5	11



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hydroperoxyte...	7.162	2.8	ug/L	52227	1	5.619	945735	50.0
Ethane, 1,1,1,2...	8.972	46.7	ug/L	1100340	2	8.850	1176980	50.0