

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111023\
 Data File : VV032894.D
 Acq On : 10 Nov 2023 16:06
 Operator : SY/MD
 Sample : 05296-04 10X
 Misc : 5.63gm/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH3R5

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\SFAMVLM103123WMA.M
 Title : VOC Analysis

Signal : TIC: VV032894.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.172	38	41	44	rBV5	1468	950	0.04%	0.006%
2	1.220	52	56	58	rBV5	2568	2087	0.09%	0.013%
3	1.278	67	74	85	rBV	198633	219740	9.34%	1.361%
4	1.523	143	150	161	rVB	180429	215933	9.18%	1.337%
5	2.056	307	316	333	rBV	368525	525918	22.36%	3.257%
6	2.253	374	377	379	rBV4	1512	939	0.04%	0.006%
7	2.336	401	403	410	rBV8	931	955	0.04%	0.006%
8	2.449	432	438	439	rBV6	3025	2994	0.13%	0.019%
9	2.545	466	468	470	rBV3	1515	968	0.04%	0.006%
10	2.603	483	486	488	rBV4	1082	833	0.04%	0.005%
11	2.613	488	489	493	rVB4	2220	1219	0.05%	0.008%
12	2.648	497	500	502	rBV4	1773	848	0.04%	0.005%
13	2.738	525	528	531	rVB5	1574	903	0.04%	0.006%
14	2.838	557	559	563	rVV5	1018	794	0.03%	0.005%
15	2.889	573	575	578	rBV4	1613	1126	0.05%	0.007%
16	2.934	586	589	592	rVB5	1608	1039	0.04%	0.006%
17	3.027	613	618	620	rBV6	1693	1316	0.06%	0.008%
18	3.082	631	635	637	rBV5	1411	1133	0.05%	0.007%
19	3.172	659	663	666	rBV6	1463	1323	0.06%	0.008%
20	3.323	707	710	713	rVV5	1267	1177	0.05%	0.007%
21	3.339	713	715	719	rVB5	1559	944	0.04%	0.006%
22	3.384	726	729	731	rBV4	1139	880	0.04%	0.005%
23	3.410	735	737	741	rBV4	1358	1020	0.04%	0.006%
24	3.452	747	750	754	rBV6	2132	1799	0.08%	0.011%
25	3.539	773	777	779	rBV5	1038	791	0.03%	0.005%
26	3.584	787	791	793	rBV4	1298	880	0.04%	0.005%
27	3.651	809	812	814	rVB4	1665	789	0.03%	0.005%
28	3.699	823	827	829	rBV6	1246	1276	0.05%	0.008%
29	3.786	845	854	875	rBV	85079	226796	9.64%	1.405%
30	4.114	955	956	961	rVV4	1275	790	0.03%	0.005%
31	4.249	981	998	1017	rBV	231237	607489	25.83%	3.762%
32	4.519	1079	1082	1084	rBV4	1549	847	0.04%	0.005%
33	4.564	1093	1096	1100	rVB6	1369	946	0.04%	0.006%
34	4.597	1100	1106	1110	rBV9	2709	2789	0.12%	0.017%
35	4.658	1123	1125	1132	rVB7	2357	2363	0.10%	0.015%
36	4.687	1132	1134	1136	rBV3	1712	794	0.03%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

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

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.M
 Title : VOC Analysis

37	4.706	1136	1140	1145	rBV7	1908	1515	0.06%	0.009%
38	4.728	1145	1147	1153	rBV6	1681	1794	0.08%	0.011%
39	4.754	1153	1155	1158	rVB4	1886	956	0.04%	0.006%
40	4.857	1185	1187	1193	rVV6	1703	1676	0.07%	0.010%
41	4.957	1202	1218	1263	rBV2	544835	1513069	64.34%	9.371%
42	5.281	1315	1319	1321	rBV5	1916	1289	0.05%	0.008%
43	5.400	1354	1356	1361	rVB6	1936	1450	0.06%	0.009%
44	5.429	1361	1365	1367	rBV5	2154	1749	0.07%	0.011%
45	5.452	1370	1372	1376	rVB5	2291	1353	0.06%	0.008%
46	5.535	1386	1398	1428	rBV	397350	877534	37.31%	5.435%
47	5.831	1478	1490	1504	rBV8	13174	34824	1.48%	0.216%
48	5.989	1526	1539	1571	rVV	311806	686103	29.17%	4.249%
49	6.252	1619	1621	1624	rBV3	1894	1073	0.05%	0.007%
50	6.368	1654	1657	1663	rVB9	1736	1520	0.06%	0.009%
51	6.445	1675	1681	1685	rBV9	1913	2252	0.10%	0.014%
52	6.561	1714	1717	1720	rVB5	1314	884	0.04%	0.005%
53	6.603	1723	1730	1736	rBV10	2654	3515	0.15%	0.022%
54	6.635	1738	1740	1744	rVB5	2302	1280	0.05%	0.008%
55	6.658	1744	1747	1749	rBV5	1216	887	0.04%	0.005%
56	6.741	1770	1773	1777	rVB6	1087	790	0.03%	0.005%
57	6.818	1794	1797	1801	rBV5	1430	1226	0.05%	0.008%
58	6.915	1814	1827	1852	rBV	166346	331924	14.11%	2.056%
59	7.121	1889	1891	1894	rBV4	2189	1105	0.05%	0.007%
60	7.143	1894	1898	1899	rBV5	1545	991	0.04%	0.006%
61	7.246	1918	1930	1967	rBV	647045	1203236	51.16%	7.452%
62	7.555	2016	2026	2050	rBV	119344	232110	9.87%	1.438%
63	7.905	2122	2135	2161	rBV	471500	835058	35.51%	5.172%
64	8.027	2163	2173	2204	rBV	304663	598881	25.46%	3.709%
65	8.285	2251	2253	2255	rBV4	1512	878	0.04%	0.005%
66	8.400	2287	2289	2291	rVB3	2174	935	0.04%	0.006%
67	8.641	2362	2364	2370	rVB8	1720	1424	0.06%	0.009%
68	8.677	2370	2375	2376	rBV5	1388	1185	0.05%	0.007%
69	8.728	2387	2391	2393	rBV5	1254	791	0.03%	0.005%
70	8.786	2398	2409	2432	rBV	674388	1137031	48.35%	7.042%
71	9.239	2549	2550	2554	rBV4	1188	929	0.04%	0.006%
72	9.384	2593	2595	2598	rBV3	1714	1095	0.05%	0.007%
73	9.571	2649	2653	2655	rBV5	2315	1772	0.08%	0.011%
74	9.699	2691	2693	2697	rVB5	1999	1216	0.05%	0.008%
75	9.735	2699	2704	2705	rBV5	1381	1089	0.05%	0.007%
76	9.844	2735	2738	2740	rBV4	1501	987	0.04%	0.006%

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 Title : VOC Analysis

77	9.857	2740	2742	2747	rVV5	3236	2777	0.12%	0.017%
78	9.879	2747	2749	2752	rVB5	1990	929	0.04%	0.006%
79	10.027	2792	2795	2796	rBV4	1399	876	0.04%	0.005%
80	10.059	2800	2805	2806	rBV5	1672	1585	0.07%	0.010%
81	10.156	2821	2835	2849	rBV	469218	746110	31.72%	4.621%
82	10.323	2881	2887	2898	rVB7	7568	11606	0.49%	0.072%
83	10.378	2901	2904	2906	rBV3	2457	1868	0.08%	0.012%
84	10.481	2934	2936	2938	rBV3	1698	948	0.04%	0.006%
85	10.657	2986	2991	2992	rBV4	2337	1985	0.08%	0.012%
86	10.821	3039	3042	3043	rBV3	1631	795	0.03%	0.005%
87	10.944	3077	3080	3081	rBV3	1711	925	0.04%	0.006%
88	11.085	3117	3124	3130	rBV3	14314	21704	0.92%	0.134%
89	11.127	3132	3137	3145	rVV	14403	20234	0.86%	0.125%
90	11.188	3145	3156	3176	rVV	721366	1135265	48.27%	7.031%
91	11.561	3261	3272	3292	rBV	777098	1228018	52.22%	7.606%
92	12.413	3531	3537	3548	rVB	17141	26671	1.13%	0.165%
93	12.587	3585	3591	3604	rVB4	24877	41817	1.78%	0.259%
94	12.882	3676	3683	3695	rVB5	37768	59335	2.52%	0.367%
95	13.075	3737	3743	3754	rVB9	16417	28436	1.21%	0.176%
96	13.201	3771	3782	3797	rBV	300594	478038	20.33%	2.961%
97	13.683	3920	3932	3948	rBV	1533167	2351829	100.00%	14.566%
98	14.448	4165	4170	4182	rVB3	30944	45427	1.93%	0.281%
99	14.760	4256	4267	4283	rVB	348480	573745	24.40%	3.553%
100	15.339	4440	4447	4460	rVB3	23994	42667	1.81%	0.264%

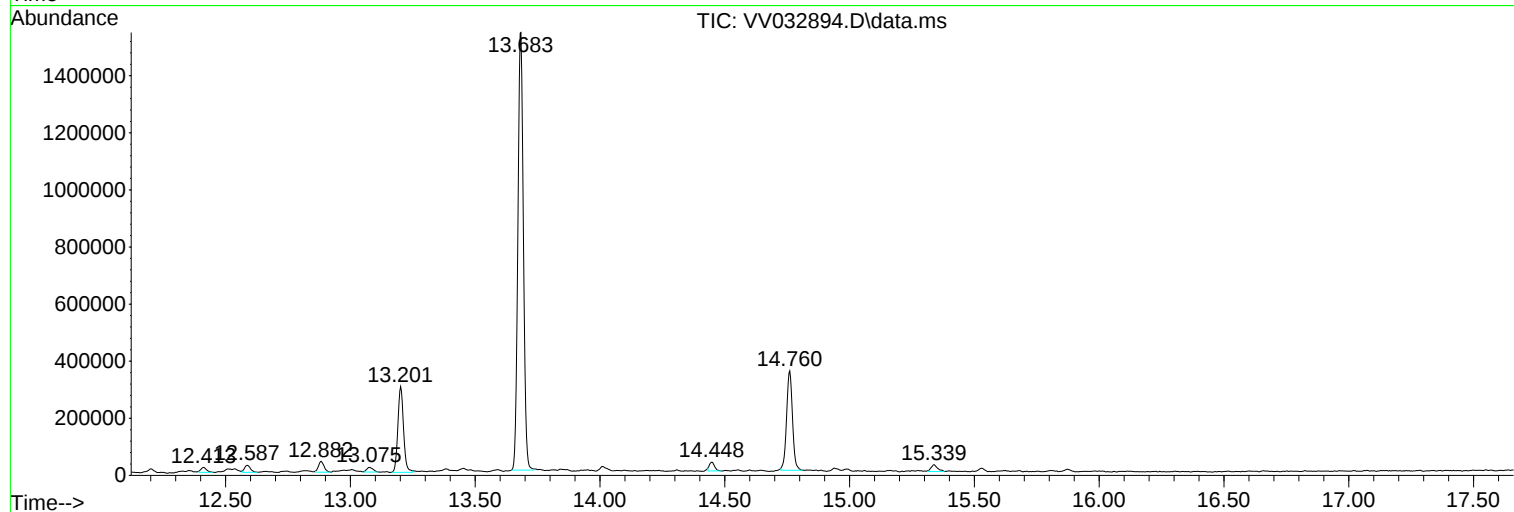
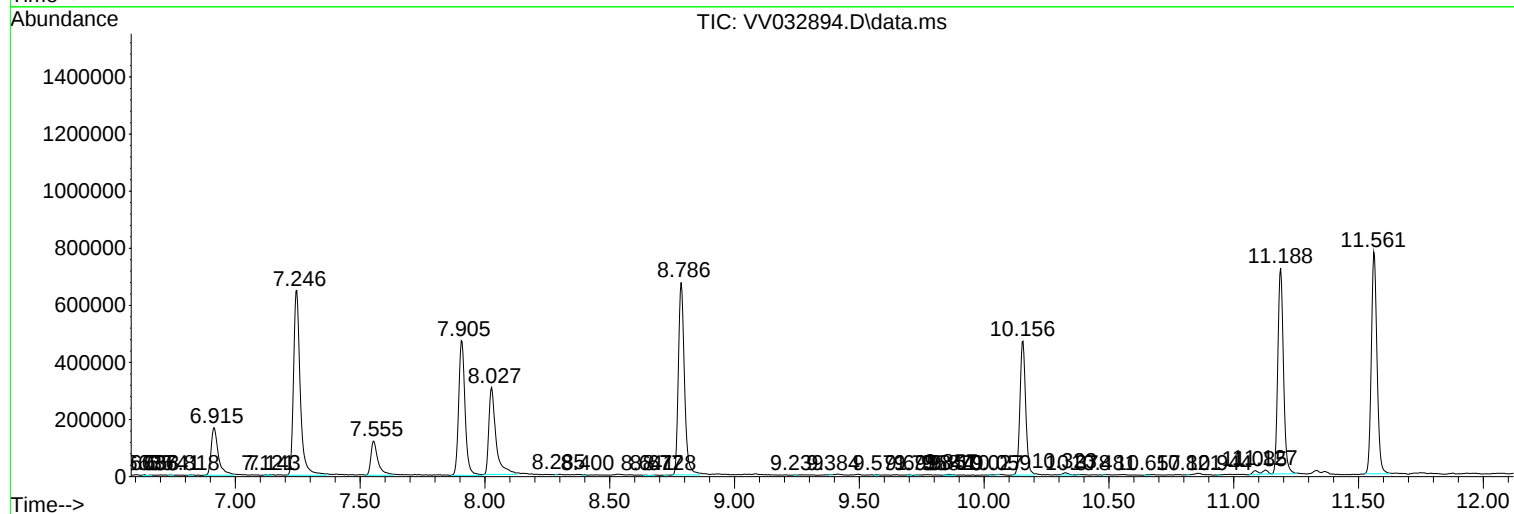
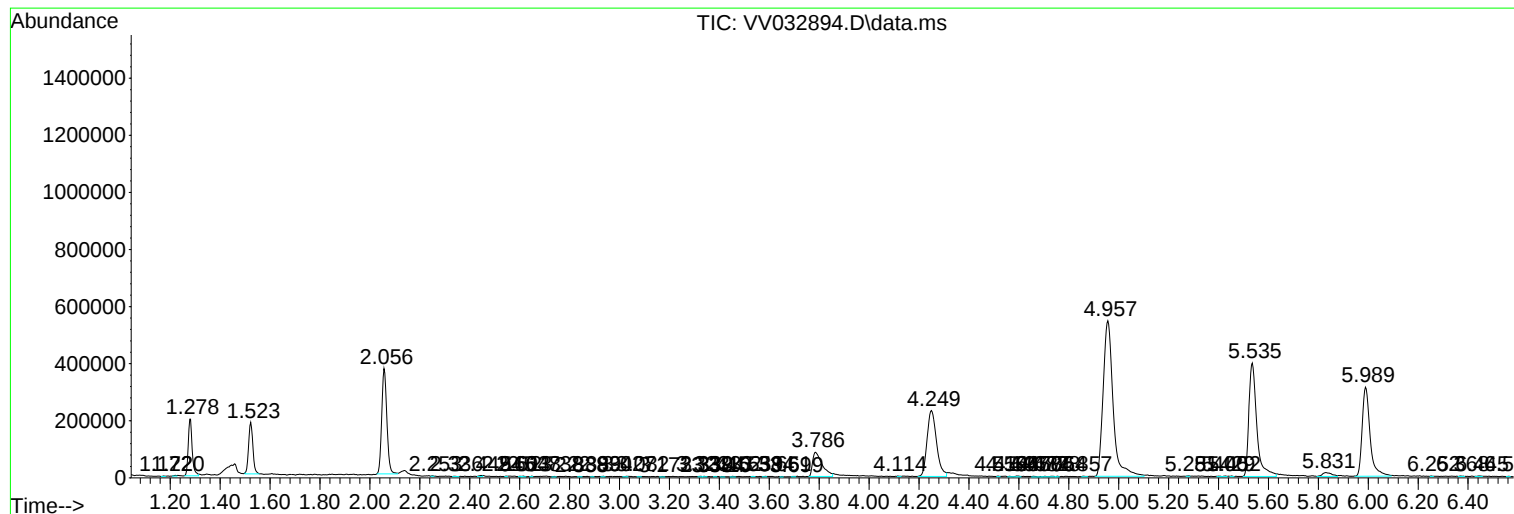
Sum of corrected areas: 16146354

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.M
Quant Title : VOC Analysis

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



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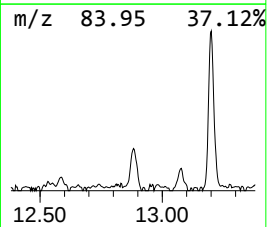
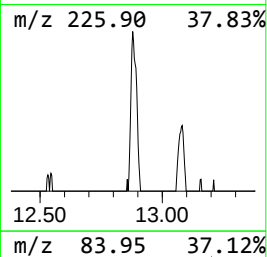
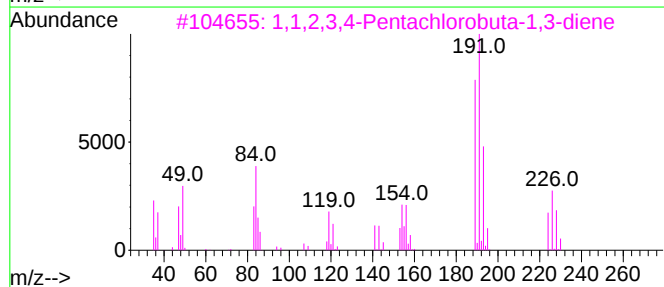
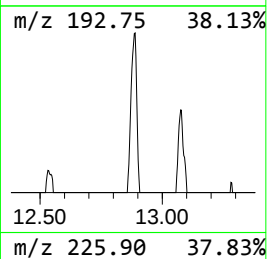
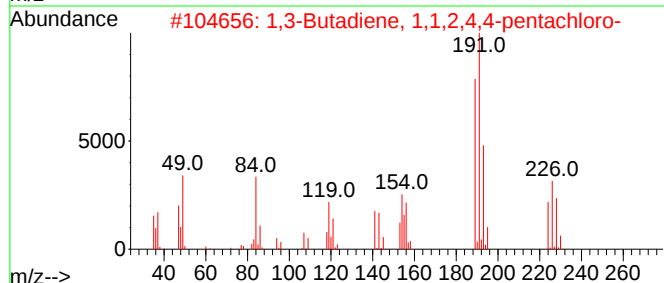
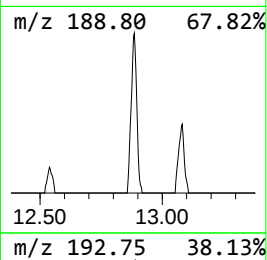
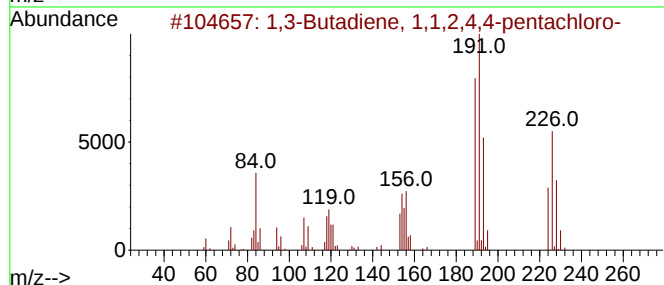
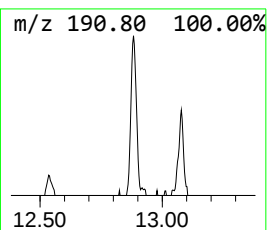
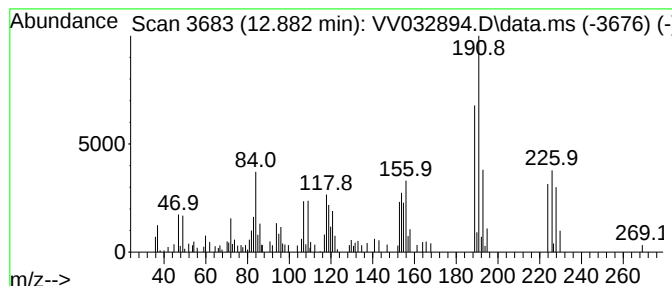
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1,3-Butadiene, 1,1,2,4,4-pe... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.882	2.61 ug/L	59335	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	98		
2	1,3-Butadiene, 1,1,2,4,4-pentach...	224	C4HCl5	021400-41-9	64		
3	1,1,2,3,4-Pentachlorobuta-1,3-diene	224	C4HCl5	1010487-10-4	46		
4	2-Thiophenecarbonyl chloride, 5-...	224	C5H2BrClOS	031555-60-9	38		
5	Thiophene-3-carbonyl chloride, 4...	224	C5H2BrClOS	072899-51-5	32		



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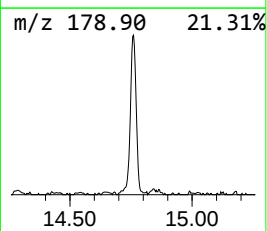
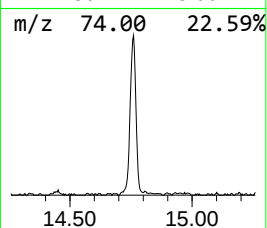
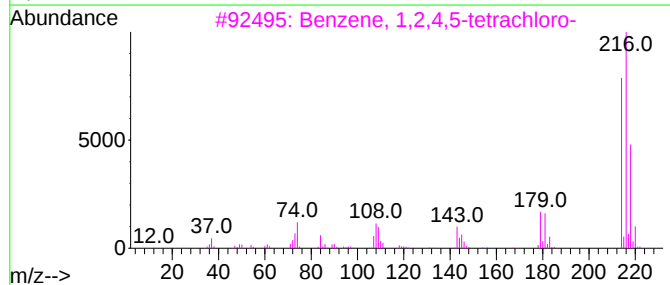
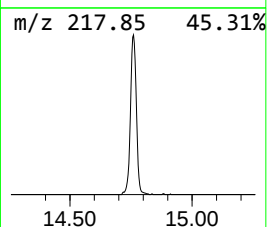
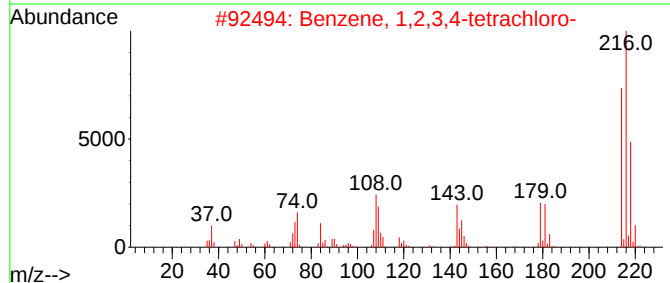
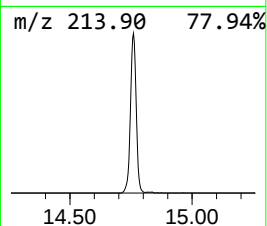
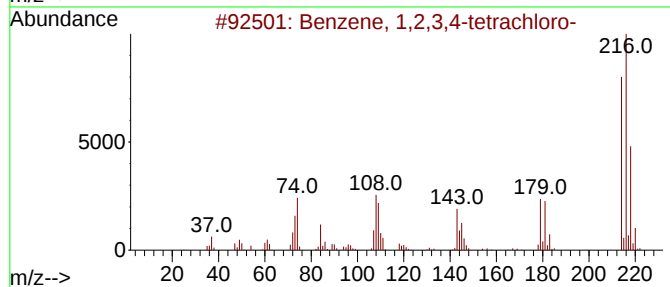
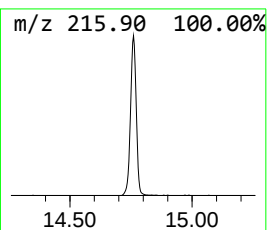
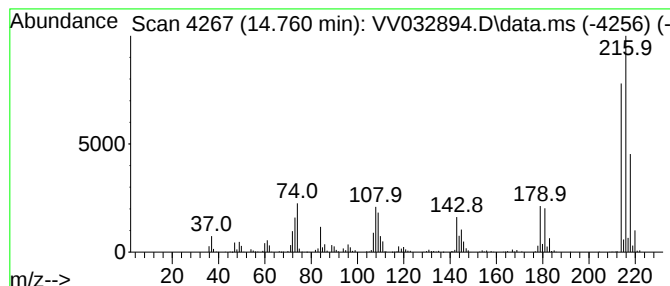
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM103123WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1,2,3,4-tetrachloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.760	25.27 ug/L	573745	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetrachloro-	214	C6H2Cl4	000634-66-2	99
2			Benzene, 1,2,3,4-tetrachloro-	214	C6H2Cl4	000634-66-2	99
3			Benzene, 1,2,4,5-tetrachloro-	214	C6H2Cl4	000095-94-3	99
4			Benzene, 1,2,4,5-tetrachloro-	214	C6H2Cl4	000095-94-3	99
5			Benzene, 1,2,3,5-tetrachloro-	214	C6H2Cl4	000634-90-2	99



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,3-Butadiene, ...	12.882	2.6	ug/L	59335	3	11.188	1135270	50.0
Benzene, 1,2,3,...	14.760	25.3	ug/L	573745	3	11.188	1135270	50.0