

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035143.D
 Acq On : 18 Apr 2023 23:24
 Operator : JC/MD
 Sample : 02397-07
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COML9

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_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035143.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.288	26	33	42	rBV	32859	104013	1.22%	0.259%
2	1.367	43	46	59	rVB	252478	287503	3.37%	0.717%
3	1.672	92	96	107	rBV	186981	249220	2.92%	0.621%
4	2.306	194	200	210	rVB	436158	684562	8.02%	1.706%
5	2.507	231	233	234	rBV2	724	416	0.00%	0.001%
6	2.544	237	239	240	rBV	431	243	0.00%	0.001%
7	2.788	276	279	284	rVV4	1057	1412	0.02%	0.004%
8	2.861	288	291	295	rVB3	538	810	0.01%	0.002%
9	2.940	303	304	308	rBV2	527	381	0.00%	0.001%
10	3.147	337	338	341	rBV3	351	289	0.00%	0.001%
11	3.221	348	350	352	rVB2	422	292	0.00%	0.001%
12	3.245	352	354	355	rBV2	337	298	0.00%	0.001%
13	3.282	359	360	363	rVV	352	211	0.00%	0.001%
14	3.349	369	371	377	rVB3	659	934	0.01%	0.002%
15	3.489	392	394	396	rVB2	411	321	0.00%	0.001%
16	3.507	396	397	399	rBV	379	305	0.00%	0.001%
17	3.556	402	405	407	rBV3	383	499	0.01%	0.001%
18	3.617	412	415	417	rBV2	401	433	0.01%	0.001%
19	3.641	417	419	421	rVV	302	230	0.00%	0.001%
20	3.696	426	428	431	rVV2	317	307	0.00%	0.001%
21	3.751	435	437	438	rBV2	256	245	0.00%	0.001%
22	3.782	440	442	445	rVB3	253	262	0.00%	0.001%
23	3.879	456	458	461	rVB2	218	232	0.00%	0.001%
24	3.928	463	466	468	rBV	308	276	0.00%	0.001%
25	3.952	468	470	471	rBV	208	215	0.00%	0.001%
26	4.062	486	488	493	rBV2	190	300	0.00%	0.001%
27	4.300	520	527	535	rVB4	1342	3884	0.05%	0.010%
28	4.458	545	553	570	rVV	122331	366334	4.29%	0.913%
29	4.733	596	598	601	rBV3	296	287	0.00%	0.001%
30	4.897	622	625	628	rVB4	335	419	0.00%	0.001%
31	4.946	628	633	634	rBV3	322	335	0.00%	0.001%
32	5.056	639	651	669	rBV	243887	782772	9.18%	1.951%
33	5.232	678	680	682	rVB3	661	372	0.00%	0.001%
34	5.342	696	698	699	rBV2	481	317	0.00%	0.001%
35	5.440	713	714	715	rBV	380	240	0.00%	0.001%
36	5.470	716	719	726	rVB4	1379	2786	0.03%	0.007%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
 Title : VOC Analysis

37	5.556	726	733	740	rBV4	1261	3455	0.04%	0.009%
38	5.671	744	752	765	rBV3	8311	24432	0.29%	0.061%
39	5.818	774	776	779	rBV2	230	262	0.00%	0.001%
40	5.970	788	801	808	rBV2	656809	1996939	23.41%	4.977%
41	6.244	844	846	848	rBV2	423	350	0.00%	0.001%
42	6.312	854	857	858	rBV2	267	270	0.00%	0.001%
43	6.452	879	880	882	rBV2	346	265	0.00%	0.001%
44	6.757	920	930	946	rBV	467644	1119624	13.12%	2.790%
45	7.110	983	988	996	rVB5	2770	6510	0.08%	0.016%
46	7.165	996	997	1001	rBV2	302	236	0.00%	0.001%
47	7.305	1011	1020	1039	rBV	405196	888930	10.42%	2.215%
48	7.567	1061	1063	1068	rVB3	494	803	0.01%	0.002%
49	7.604	1068	1069	1072	rBV2	358	396	0.00%	0.001%
50	7.769	1094	1096	1098	rVV	356	231	0.00%	0.001%
51	7.878	1113	1114	1116	rVB	391	208	0.00%	0.001%
52	7.897	1116	1117	1119	rBV2	340	251	0.00%	0.001%
53	7.945	1119	1125	1132	rVV3	1633	3290	0.04%	0.008%
54	8.061	1141	1144	1147	rVB3	414	532	0.01%	0.001%
55	8.116	1151	1153	1159	rVB5	977	1290	0.02%	0.003%
56	8.323	1180	1187	1202	rBV	261979	428876	5.03%	1.069%
57	8.494	1212	1215	1217	rBV2	1036	975	0.01%	0.002%
58	8.646	1234	1240	1253	rBV	1041795	1624954	19.05%	4.050%
59	8.896	1277	1281	1284	rBV3	501	515	0.01%	0.001%
60	8.951	1284	1290	1301	rBV	180903	274333	3.22%	0.684%
61	9.140	1319	1321	1323	rVB	542	305	0.00%	0.001%
62	9.274	1340	1343	1348	rVB3	2848	3284	0.04%	0.008%
63	9.329	1350	1352	1355	rBV3	328	331	0.00%	0.001%
64	9.384	1355	1361	1374	rBV	591921	827324	9.70%	2.062%
65	10.079	1465	1475	1490	rBV2	4341537	7033701	82.44%	17.529%
66	10.963	1618	1620	1621	rBV2	490	323	0.00%	0.001%
67	11.006	1625	1627	1628	rBV2	447	376	0.00%	0.001%
68	11.189	1652	1657	1670	rBV	637476	853859	10.01%	2.128%
69	11.366	1684	1686	1692	rVB3	1923	2188	0.03%	0.005%
70	11.548	1715	1716	1718	rBV	342	277	0.00%	0.001%
71	11.573	1718	1720	1721	rVV	338	255	0.00%	0.001%
72	11.591	1721	1723	1725	rVV3	451	468	0.01%	0.001%
73	11.707	1735	1742	1746	rBV5	930	1667	0.02%	0.004%
74	11.969	1780	1785	1789	rBV	1928357	2380405	27.90%	5.932%
75	12.042	1789	1797	1805	rVB2	4738096	6958841	81.57%	17.343%
76	12.219	1823	1826	1830	rBV2	7395	10579	0.12%	0.026%

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Min Area: 0 % of largest Peak

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77	12.335	1837	1845	1852	rBV2	6113317	8531411	100.00%	21.262%
78	12.664	1896	1899	1900	rBV2	665	680	0.01%	0.002%
79	12.920	1937	1941	1951	rBV2	8163	12232	0.14%	0.030%
80	13.060	1960	1964	1968	rBV4	3831	6668	0.08%	0.017%
81	13.109	1969	1972	1980	rVV3	5680	8383	0.10%	0.021%
82	13.201	1982	1987	1991	rVB	5989	8144	0.10%	0.020%
83	13.237	1991	1993	1995	rBV2	268	210	0.00%	0.001%
84	13.274	1998	1999	2000	rBV2	340	203	0.00%	0.001%
85	13.322	2006	2007	2010	rBV2	274	279	0.00%	0.001%
86	13.469	2030	2031	2032	rBV	314	224	0.00%	0.001%
87	13.518	2036	2039	2040	rBV	396	441	0.01%	0.001%
88	13.585	2045	2050	2069	rVB	2388019	2952916	34.61%	7.359%
89	13.963	2106	2112	2125	rVB	816329	1078837	12.65%	2.689%
90	14.261	2159	2161	2165	rBV3	1370	1580	0.02%	0.004%
91	14.456	2192	2193	2194	rBV	528	263	0.00%	0.001%
92	14.621	2218	2220	2222	rBV3	1124	1055	0.01%	0.003%
93	14.664	2225	2227	2229	rVV3	582	451	0.01%	0.001%
94	14.719	2235	2236	2238	rBV2	557	236	0.00%	0.001%
95	14.780	2239	2246	2253	rVB	73104	123335	1.45%	0.307%
96	15.097	2296	2298	2299	rBV2	545	371	0.00%	0.001%
97	15.249	2317	2323	2337	rVB	301450	434473	5.09%	1.083%
98	15.346	2337	2339	2340	rBV2	673	485	0.01%	0.001%
99	15.859	2421	2423	2424	rVB	773	302	0.00%	0.001%
100	16.505	2525	2529	2535	rVB4	10753	18247	0.21%	0.045%

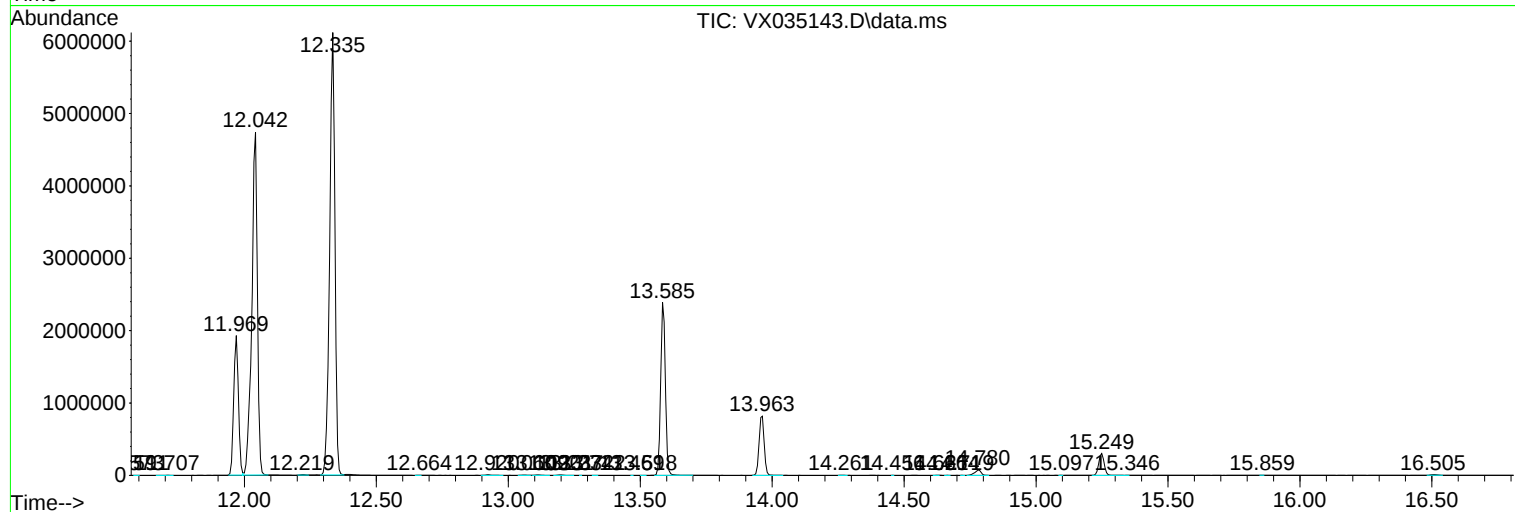
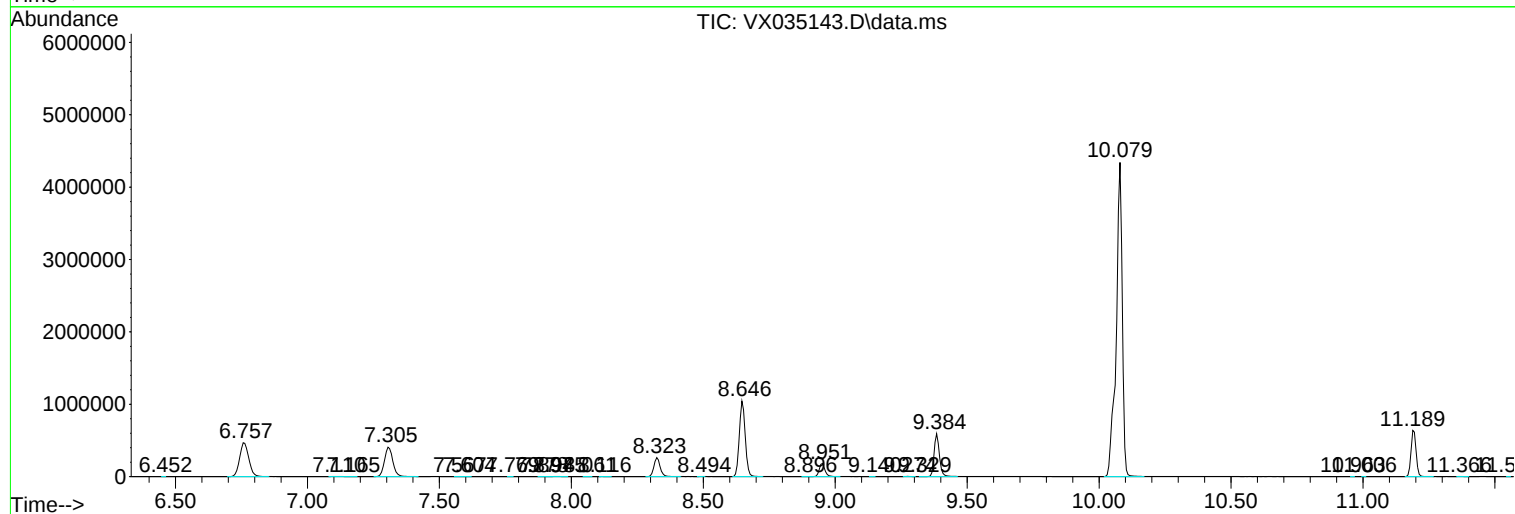
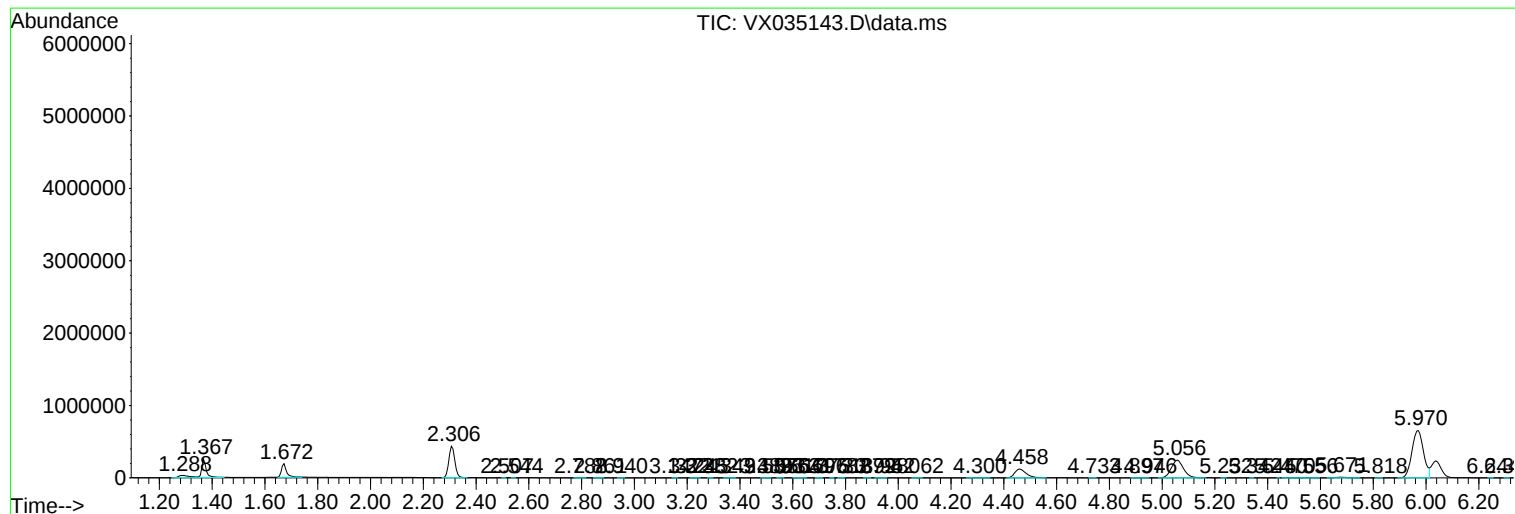
Sum of corrected areas: 40125491

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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



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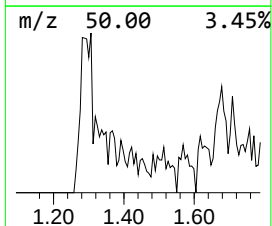
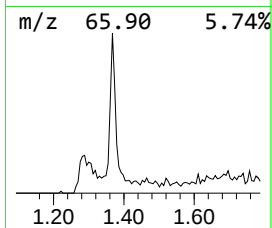
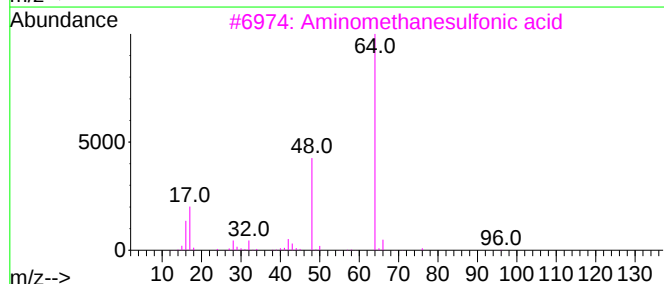
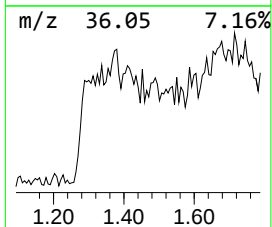
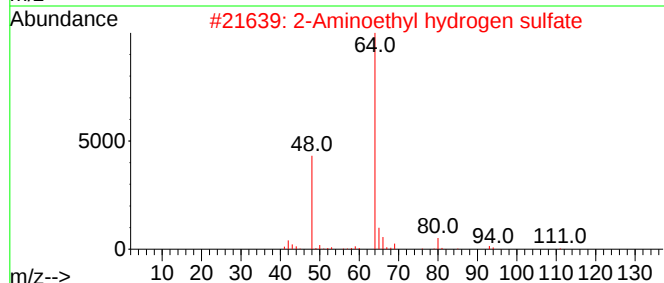
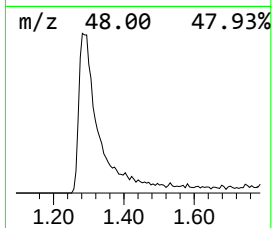
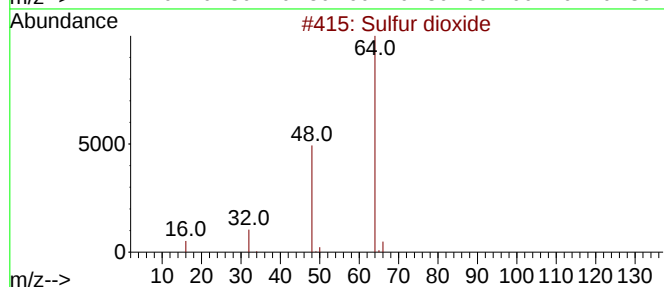
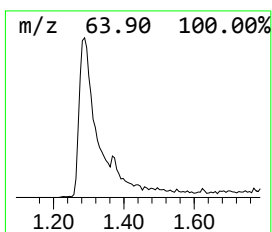
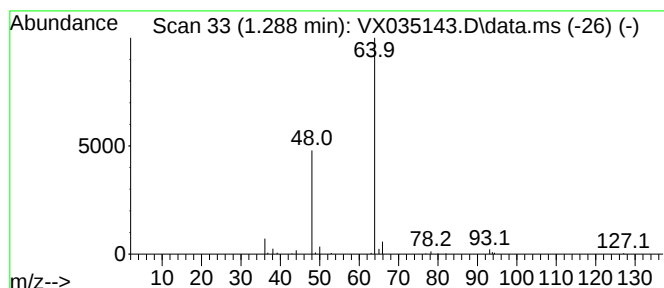
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.288	4.64 ug/L	104013	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	83
3			Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	64
4			Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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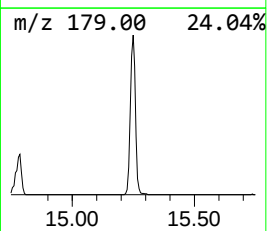
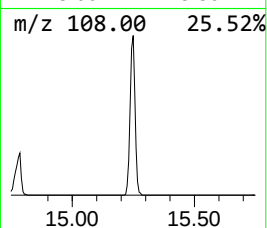
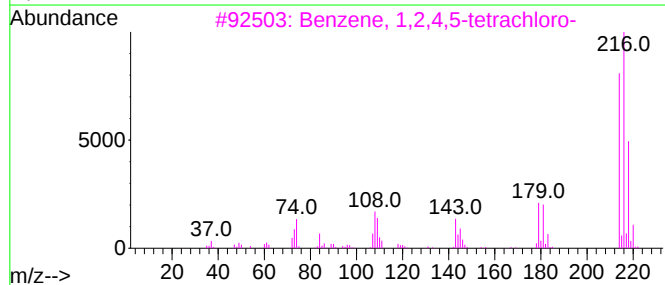
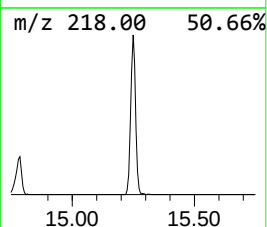
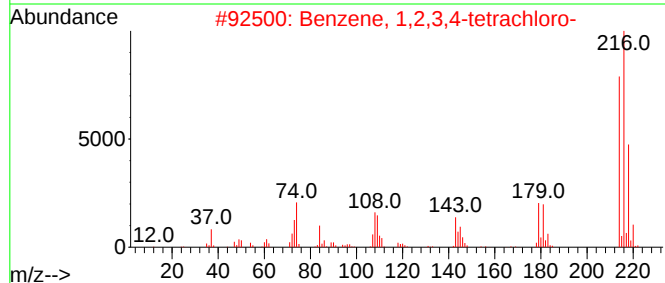
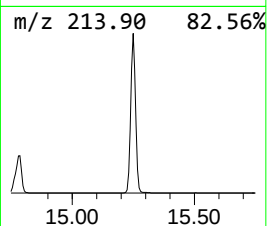
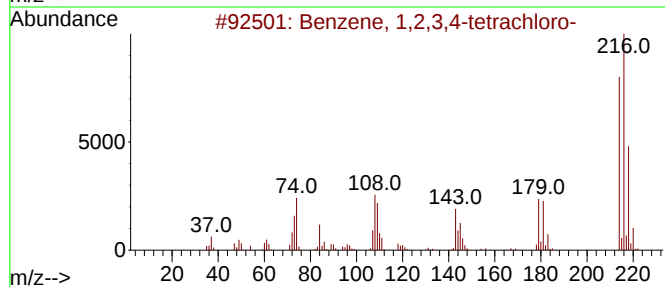
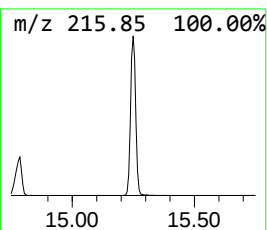
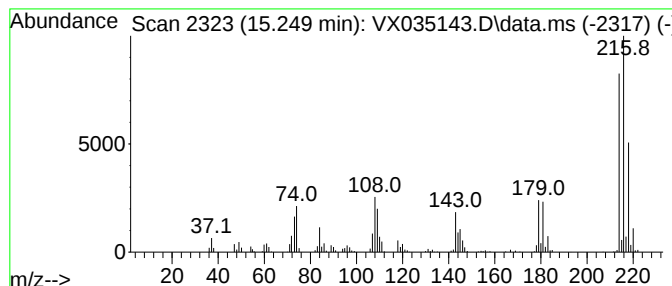
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.249	3.12 ug/L	434473	1,4-Dichlorobenzene-d4	12.024

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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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.288	4.6	ug/L	104013	1	6.757	1119620	50.0
Benzene, 1,2,3,...	15.249	3.1	ug/L	434473	3	12.024	6958840	50.0