

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035145.D
 Acq On : 19 Apr 2023 00:11
 Operator : JC/MD
 Sample : 02397-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM1

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: VX035145.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	15	rVB4	1021	1405	0.00%	0.001%
2	1.295	25	34	42	rBV	27440	76872	0.15%	0.061%
3	1.368	42	46	58	rVB	258628	290076	0.58%	0.231%
4	1.673	91	96	109	rVB	174343	230327	0.46%	0.183%
5	2.307	193	200	209	rBV	448210	696359	1.39%	0.555%
6	2.392	209	214	226	rVB	20782	45052	0.09%	0.036%
7	2.514	231	234	237	rBV4	442	515	0.00%	0.000%
8	2.593	239	247	248	rBV	3742	7226	0.01%	0.006%
9	2.794	274	280	282	rBV6	723	1249	0.00%	0.001%
10	2.855	288	290	292	rBV	276	349	0.00%	0.000%
11	2.995	309	313	314	rBV3	380	435	0.00%	0.000%
12	3.233	348	352	355	rVV2	452	375	0.00%	0.000%
13	3.629	416	417	421	rVB2	280	351	0.00%	0.000%
14	3.684	421	426	429	rBV3	243	403	0.00%	0.000%
15	4.257	516	520	521	rVV3	279	365	0.00%	0.000%
16	4.312	521	529	532	rVV6	1564	3563	0.01%	0.003%
17	4.459	544	553	574	rBV	124213	379361	0.76%	0.302%
18	5.056	638	651	669	rBV2	245770	756591	1.51%	0.603%
19	5.227	677	679	683	rVB3	618	814	0.00%	0.001%
20	5.263	683	685	687	rBV2	402	390	0.00%	0.000%
21	5.379	702	704	706	rBV	365	372	0.00%	0.000%
22	5.477	718	720	726	rVB3	787	1483	0.00%	0.001%
23	5.550	726	732	733	rBV4	900	1652	0.00%	0.001%
24	5.562	733	734	737	rVB2	681	386	0.00%	0.000%
25	5.739	761	763	768	rVB3	253	353	0.00%	0.000%
26	5.971	787	801	808	rBV2	672457	2052047	4.09%	1.634%
27	6.038	808	812	836	rVB	276348	676819	1.35%	0.539%
28	6.361	861	865	868	rBV	406	447	0.00%	0.000%
29	6.757	920	930	949	rBV	475255	1145320	2.28%	0.912%
30	7.111	983	988	996	rBV5	2643	6445	0.01%	0.005%
31	7.226	1004	1007	1009	rBV3	459	628	0.00%	0.001%
32	7.306	1011	1020	1044	rVV	409957	904831	1.80%	0.721%
33	7.489	1044	1050	1053	rVV5	1401	3070	0.01%	0.002%
34	7.537	1056	1058	1060	rVV2	472	397	0.00%	0.000%
35	7.946	1119	1125	1126	rBV5	1550	2521	0.01%	0.002%
36	8.037	1137	1140	1142	rBV3	315	371	0.00%	0.000%

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37	8.238	1170	1173	1175	rBV3	324	487	0.00%	0.000%
38	8.324	1180	1187	1199	rBV	256409	418878	0.84%	0.334%
39	8.488	1211	1214	1217	rBV3	977	1316	0.00%	0.001%
40	8.647	1233	1240	1259	rVV	1079801	1671332	3.33%	1.331%
41	8.866	1274	1276	1281	rVB4	351	526	0.00%	0.000%
42	8.952	1284	1290	1304	rBV	176773	269830	0.54%	0.215%
43	9.159	1322	1324	1327	rVB3	375	386	0.00%	0.000%
44	9.275	1339	1343	1349	rVB3	1932	2550	0.01%	0.002%
45	9.385	1355	1361	1376	rBV	582739	832879	1.66%	0.663%
46	9.659	1405	1406	1410	rVB3	405	421	0.00%	0.000%
47	9.714	1413	1415	1418	rVB5	647	812	0.00%	0.001%
48	9.763	1421	1423	1425	rVB3	465	358	0.00%	0.000%
49	10.080	1465	1475	1500	rBV	17009927	25027626	49.91%	19.933%
50	10.299	1509	1511	1514	rVB4	721	797	0.00%	0.001%
51	10.439	1533	1534	1540	rVB5	763	1066	0.00%	0.001%
52	10.701	1573	1577	1580	rBV2	555	880	0.00%	0.001%
53	10.970	1616	1621	1623	rVB2	459	662	0.00%	0.001%
54	11.189	1652	1657	1667	rBV	661184	858748	1.71%	0.684%
55	11.311	1673	1677	1681	rVB4	993	1573	0.00%	0.001%
56	11.360	1681	1685	1692	rBV4	2660	3796	0.01%	0.003%
57	11.457	1695	1701	1707	rBV3	817	1352	0.00%	0.001%
58	11.707	1740	1742	1745	rVB3	956	722	0.00%	0.001%
59	11.756	1747	1750	1752	rBV2	643	756	0.00%	0.001%
60	11.890	1771	1772	1775	rVB3	455	390	0.00%	0.000%
61	11.969	1779	1785	1789	rBV	2172966	2618944	5.22%	2.086%
62	12.043	1789	1797	1806	rVB2	8988012	12448243	24.82%	9.914%
63	12.219	1822	1826	1834	rBV3	8689	16535	0.03%	0.013%
64	12.341	1837	1846	1851	rBV	35225142	50147523	100.00%	39.940%
65	12.603	1887	1889	1891	rBV2	763	861	0.00%	0.001%
66	12.701	1901	1905	1910	rVB5	2211	2989	0.01%	0.002%
67	12.878	1926	1934	1936	rBV5	3005	5420	0.01%	0.004%
68	12.921	1936	1941	1950	rVB	147077	185392	0.37%	0.148%
69	13.061	1957	1964	1969	rBV	54174	102646	0.20%	0.082%
70	13.110	1969	1972	1978	rVV	15600	20659	0.04%	0.016%
71	13.195	1980	1986	1996	rBV	68983	92402	0.18%	0.074%
72	13.353	2010	2012	2013	rBV2	405	380	0.00%	0.000%
73	13.384	2013	2017	2021	rVV2	11032	14754	0.03%	0.012%
74	13.427	2021	2024	2026	rVB3	399	452	0.00%	0.000%
75	13.591	2045	2051	2064	rVB	14491695	18293145	36.48%	14.569%
76	13.780	2078	2082	2087	rVB	7273	9594	0.02%	0.008%

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77	13.841	2090	2092	2093	rBV	512	418	0.00%	0.000%
78	13.963	2106	2112	2129	rVB	3065516	3840237	7.66%	3.059%
79	14.213	2151	2153	2156	rBV4	524	398	0.00%	0.000%
80	14.286	2164	2165	2170	rVB5	516	787	0.00%	0.001%
81	14.384	2176	2181	2185	rBV4	3908	7223	0.01%	0.006%
82	14.542	2203	2207	2210	rBV3	5100	5960	0.01%	0.005%
83	14.628	2216	2221	2229	rVB5	7934	13014	0.03%	0.010%
84	14.682	2229	2230	2234	rBV	695	747	0.00%	0.001%
85	14.780	2234	2246	2253	rBV	212563	330395	0.66%	0.263%
86	14.926	2265	2270	2273	rBV3	2487	2763	0.01%	0.002%
87	15.091	2295	2297	2299	rVB3	478	348	0.00%	0.000%
88	15.115	2299	2301	2302	rBV	417	370	0.00%	0.000%
89	15.249	2316	2323	2336	rVV	686093	951446	1.90%	0.758%
90	15.518	2365	2367	2370	rVB2	553	436	0.00%	0.000%
91	15.585	2377	2378	2380	rBV2	887	759	0.00%	0.001%
92	15.737	2401	2403	2404	rVB2	691	371	0.00%	0.000%
93	16.030	2447	2451	2456	rBV4	568	1258	0.00%	0.001%
94	16.072	2456	2458	2460	rVB3	570	426	0.00%	0.000%
95	16.188	2475	2477	2479	rVB2	702	514	0.00%	0.000%
96	16.310	2493	2497	2498	rBV3	781	900	0.00%	0.001%
97	16.426	2515	2516	2518	rBV2	647	426	0.00%	0.000%
98	16.505	2523	2529	2536	rBV3	26028	50838	0.10%	0.040%
99	16.633	2548	2550	2553	rVB4	659	567	0.00%	0.000%
100	16.749	2567	2569	2570	rVB2	726	442	0.00%	0.000%

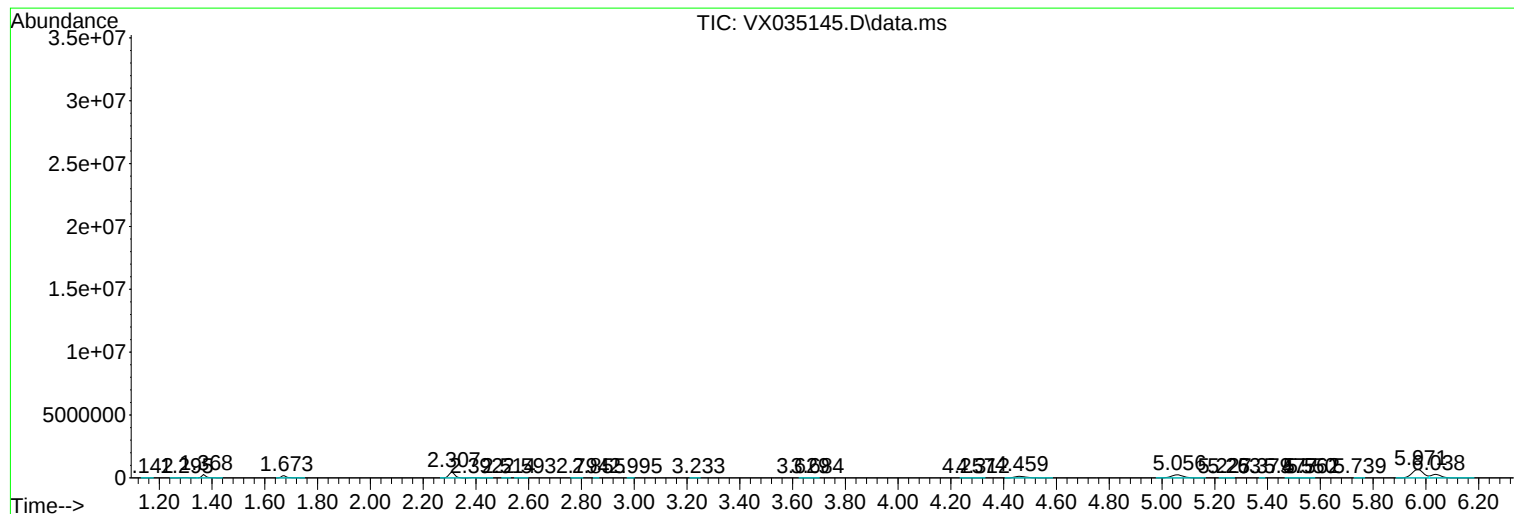
Sum of corrected areas: 125558345

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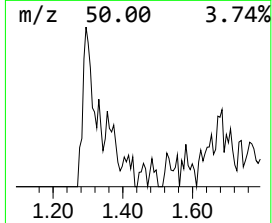
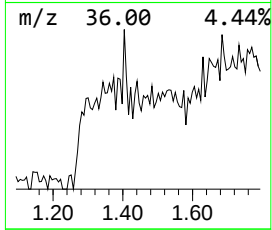
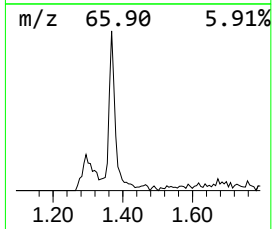
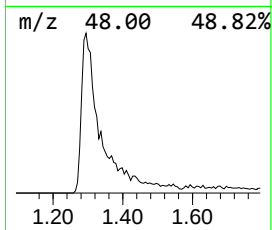
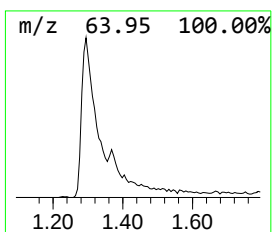
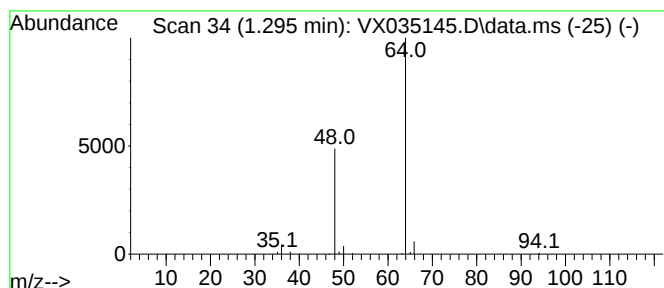
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.295	3.36 ug/L	76872	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Sulfur dioxide	64	O2S	007446-09-5	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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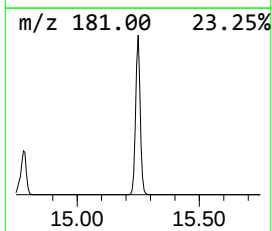
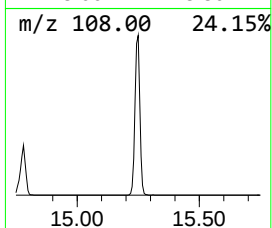
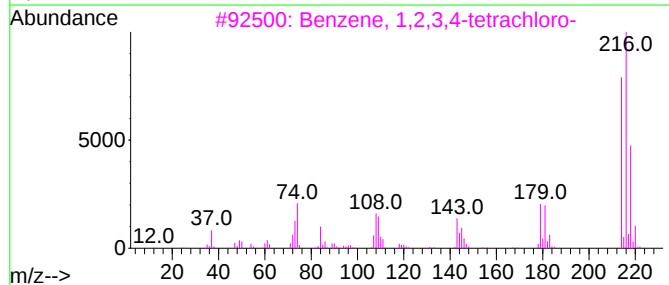
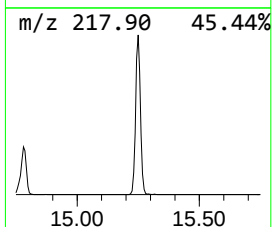
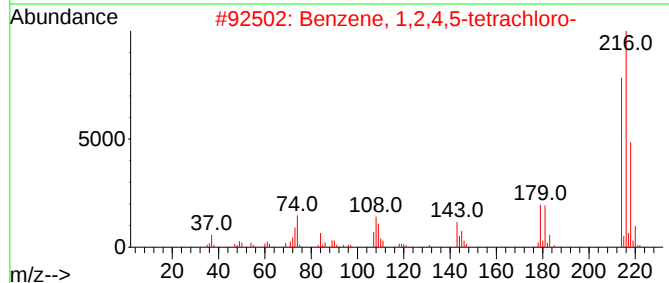
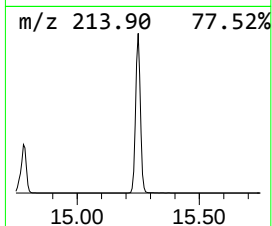
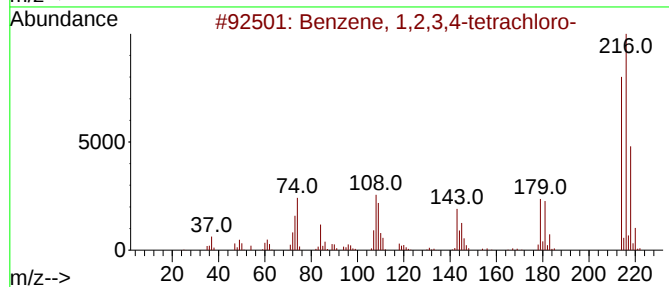
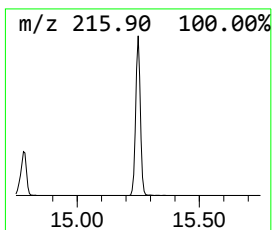
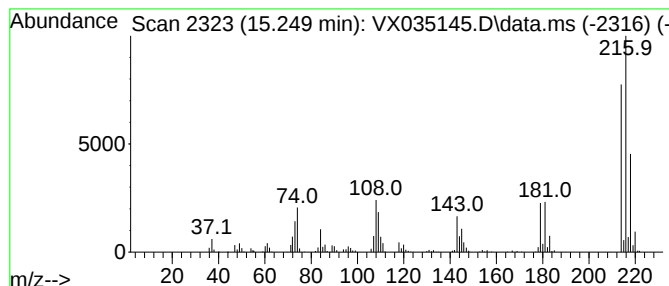
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM041823WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.249	3.82 ug/L	951446	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, 1,2,4,5-tetrachloro-	214	C6H2Cl4	000095-94-3	99
3			Benzene, 1,2,3,4-tetrachloro-	214	C6H2Cl4	000634-66-2	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\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.295	3.4	ug/L	76872	1	6.763	1145320	50.0
Benzene, 1,2,3,...	15.249	3.8	ug/L	951446	3	12.024	12448200	50.0