

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035140.D
 Acq On : 18 Apr 2023 22:15
 Operator : JC/MD
 Sample : 02397-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COML6

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: VX035140.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	24	31	42	rBV	43460	144753	1.99%	0.382%
2	1.368	42	46	58	rVB	250043	277749	3.82%	0.733%
3	1.672	92	96	107	rVB	175613	232592	3.20%	0.614%
4	2.306	194	200	210	rBV	457610	713808	9.82%	1.884%
5	2.782	275	278	279	rBV3	837	823	0.01%	0.002%
6	2.855	288	290	291	rBV	263	200	0.00%	0.001%
7	2.940	299	304	310	rVB2	1320	2923	0.04%	0.008%
8	3.099	328	330	331	rBV2	402	361	0.00%	0.001%
9	3.312	363	365	366	rBV2	251	204	0.00%	0.001%
10	3.331	366	368	371	rBV3	207	207	0.00%	0.001%
11	3.361	371	373	375	rBV3	182	192	0.00%	0.001%
12	3.410	379	381	382	rBV2	195	198	0.00%	0.001%
13	3.629	412	417	418	rBV3	313	410	0.01%	0.001%
14	3.696	426	428	433	rVB3	192	270	0.00%	0.001%
15	3.763	438	439	442	rBV2	386	357	0.00%	0.001%
16	3.971	471	473	475	rBV	177	218	0.00%	0.001%
17	4.032	481	483	485	rVB	365	270	0.00%	0.001%
18	4.056	485	487	488	rBV	337	209	0.00%	0.001%
19	4.099	492	494	497	rBV2	315	328	0.00%	0.001%
20	4.141	499	501	502	rBV2	221	215	0.00%	0.001%
21	4.300	519	527	532	rVB5	580	1777	0.02%	0.005%
22	4.355	534	536	538	rVB2	331	183	0.00%	0.000%
23	4.458	544	553	573	rBV	126274	375974	5.17%	0.992%
24	4.782	604	606	607	rVB2	514	277	0.00%	0.001%
25	5.056	639	651	671	rBV	250475	806498	11.09%	2.129%
26	5.367	699	702	703	rBV	449	380	0.01%	0.001%
27	5.470	715	719	726	rBV4	620	998	0.01%	0.003%
28	5.537	726	730	731	rBV3	875	840	0.01%	0.002%
29	5.684	744	754	764	rBV3	4120	11893	0.16%	0.031%
30	5.781	768	770	771	rBV2	296	245	0.00%	0.001%
31	5.970	789	801	807	rBV2	680227	2061067	28.34%	5.441%
32	6.324	856	859	861	rBV2	197	276	0.00%	0.001%
33	6.348	861	863	866	rVB2	427	279	0.00%	0.001%
34	6.391	868	870	873	rBV2	410	510	0.01%	0.001%
35	6.537	891	894	895	rBV2	293	257	0.00%	0.001%
36	6.592	901	903	907	rVB3	328	282	0.00%	0.001%

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

37	6.647	911	912	915	rVB2	218	200	0.00%	0.001%
38	6.763	919	931	949	rBV	475754	1153479	15.86%	3.045%
39	7.110	982	988	996	rVV6	2293	5784	0.08%	0.015%
40	7.220	1004	1006	1007	rBV	428	300	0.00%	0.001%
41	7.238	1007	1009	1011	rBV	271	199	0.00%	0.001%
42	7.305	1011	1020	1034	rBV	414127	911737	12.54%	2.407%
43	7.476	1044	1048	1049	rBV3	1170	1348	0.02%	0.004%
44	7.738	1089	1091	1092	rBV2	211	180	0.00%	0.000%
45	7.848	1106	1109	1111	rBV2	345	294	0.00%	0.001%
46	7.897	1115	1117	1120	rVB2	259	234	0.00%	0.001%
47	7.946	1120	1125	1132	rBV4	1783	3625	0.05%	0.010%
48	8.068	1143	1145	1147	rVB2	231	200	0.00%	0.001%
49	8.232	1170	1172	1175	rBV2	303	402	0.01%	0.001%
50	8.275	1178	1179	1181	rBV	253	244	0.00%	0.001%
51	8.324	1181	1187	1198	rBV	254888	423416	5.82%	1.118%
52	8.647	1233	1240	1260	rBV	1099917	1675654	23.04%	4.423%
53	8.952	1284	1290	1308	rBV	174264	270291	3.72%	0.714%
54	9.116	1315	1317	1320	rBV	346	408	0.01%	0.001%
55	9.165	1323	1325	1329	rBV3	344	412	0.01%	0.001%
56	9.275	1339	1343	1349	rVB6	3082	4711	0.06%	0.012%
57	9.384	1356	1361	1372	rBV	592071	828472	11.39%	2.187%
58	10.000	1460	1462	1465	rBV	252	298	0.00%	0.001%
59	10.079	1465	1475	1498	rVV2	4373856	7090455	97.51%	18.717%
60	10.299	1509	1511	1512	rBV2	604	264	0.00%	0.001%
61	10.659	1569	1570	1573	rBV	379	369	0.01%	0.001%
62	10.695	1574	1576	1578	rVB2	406	298	0.00%	0.001%
63	10.829	1597	1598	1603	rBV3	225	340	0.00%	0.001%
64	11.061	1635	1636	1637	rBV	303	181	0.00%	0.000%
65	11.091	1640	1641	1643	rVB	367	210	0.00%	0.001%
66	11.189	1652	1657	1669	rBV	666381	872469	12.00%	2.303%
67	11.311	1674	1677	1683	rVB4	705	1074	0.01%	0.003%
68	11.366	1683	1686	1690	rBV2	1195	1686	0.02%	0.004%
69	11.457	1699	1701	1705	rVB4	719	800	0.01%	0.002%
70	11.543	1713	1715	1718	rVB2	277	229	0.00%	0.001%
71	11.610	1724	1726	1728	rBV2	257	240	0.00%	0.001%
72	11.683	1737	1738	1740	rVB	441	196	0.00%	0.001%
73	11.707	1740	1742	1745	rVB3	956	830	0.01%	0.002%
74	11.756	1749	1750	1751	rBV	410	214	0.00%	0.001%
75	11.969	1779	1785	1789	rBV	1236179	1505615	20.71%	3.974%
76	12.042	1789	1797	1806	rVB2	4043771	6237504	85.78%	16.466%

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Integrator: RTE

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Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

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

77	12.219	1823	1826	1833	rBV3	4260	6487	0.09%	0.017%
78	12.335	1837	1845	1858	rBV2	4951563	7271605	100.00%	19.195%
79	12.658	1894	1898	1901	rBV3	533	955	0.01%	0.003%
80	12.707	1901	1906	1908	rBV5	760	1158	0.02%	0.003%
81	12.920	1938	1941	1946	rBV2	5918	8253	0.11%	0.022%
82	13.006	1954	1955	1956	rBV	354	189	0.00%	0.000%
83	13.024	1956	1958	1959	rVV	409	235	0.00%	0.001%
84	13.061	1961	1964	1969	rVV5	1741	2881	0.04%	0.008%
85	13.109	1969	1972	1979	rVB5	3846	5419	0.07%	0.014%
86	13.195	1983	1986	1992	rVB3	3943	5140	0.07%	0.014%
87	13.237	1992	1993	1995	rBV	311	210	0.00%	0.001%
88	13.298	2002	2003	2005	rVB	343	219	0.00%	0.001%
89	13.426	2021	2024	2025	rBV	252	216	0.00%	0.001%
90	13.585	2045	2050	2074	rVB	2395309	3006954	41.35%	7.938%
91	13.780	2080	2082	2085	rVB2	1084	977	0.01%	0.003%
92	13.841	2090	2092	2095	rBV2	405	346	0.00%	0.001%
93	13.963	2106	2112	2121	rVB	466340	595555	8.19%	1.572%
94	14.213	2151	2153	2158	rBV2	397	565	0.01%	0.001%
95	14.329	2170	2172	2174	rBV2	372	293	0.00%	0.001%
96	14.383	2175	2181	2189	rVB3	4135	7040	0.10%	0.019%
97	14.780	2239	2246	2256	rVB2	92488	182502	2.51%	0.482%
98	14.853	2256	2258	2259	rBV	527	410	0.01%	0.001%
99	15.249	2316	2323	2337	rVB	808838	1125576	15.48%	2.971%
100	16.511	2525	2530	2538	rVB3	13793	25875	0.36%	0.068%

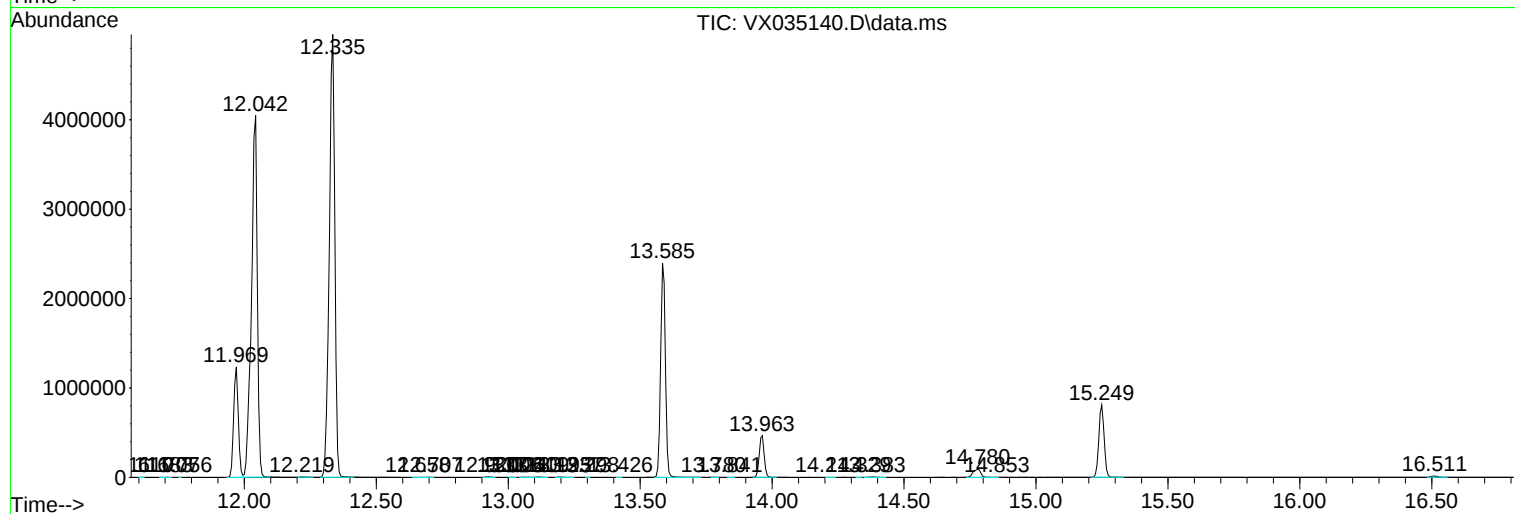
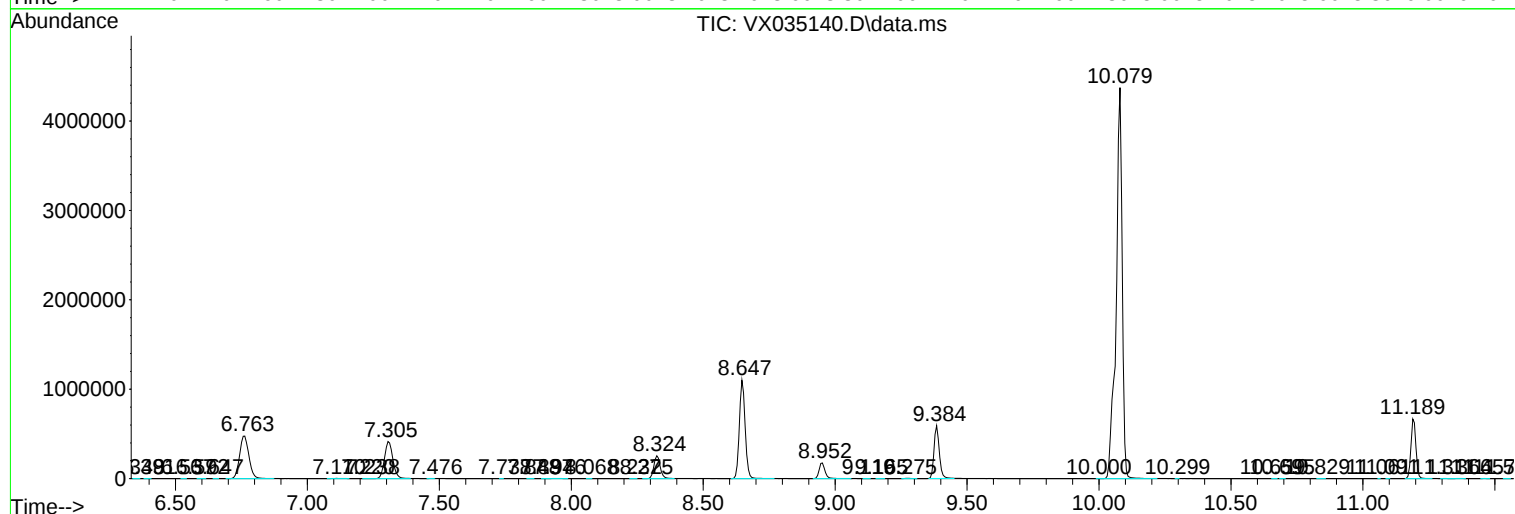
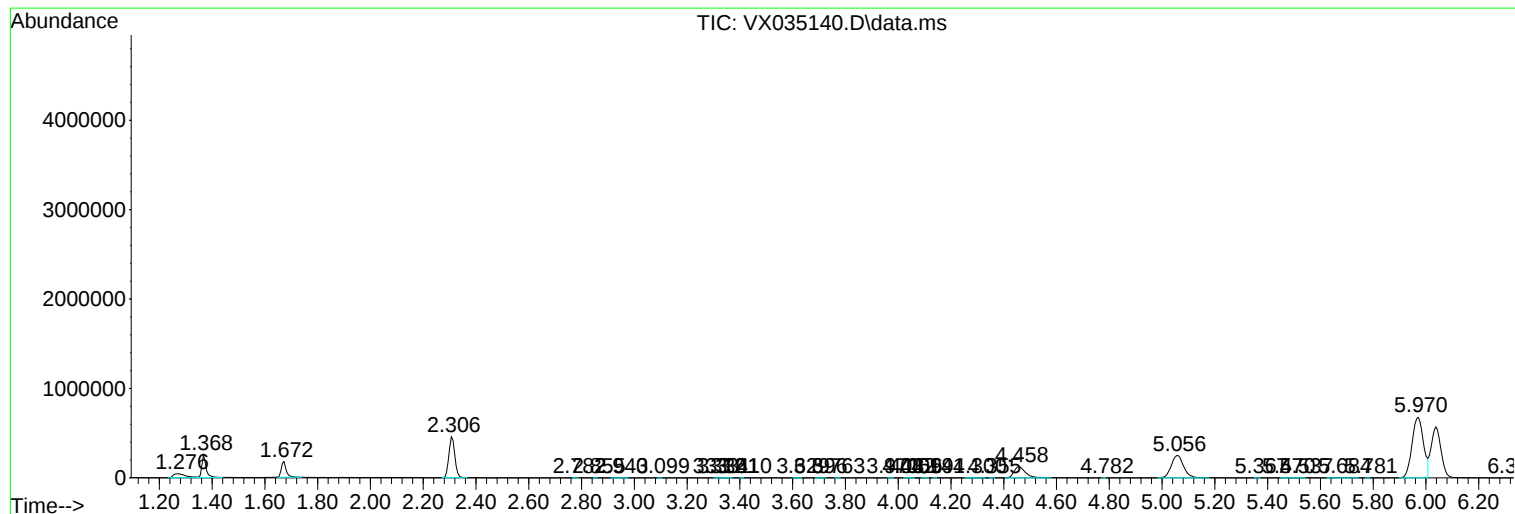
Sum of corrected areas: 37881945

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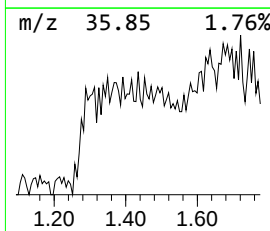
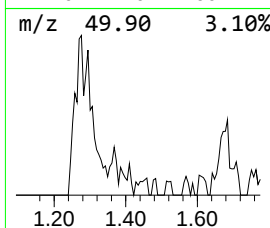
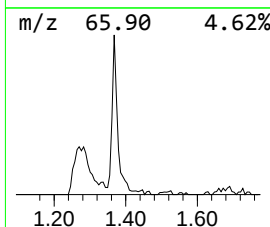
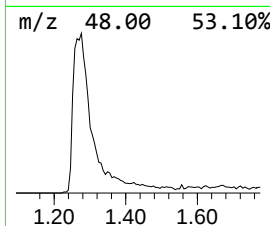
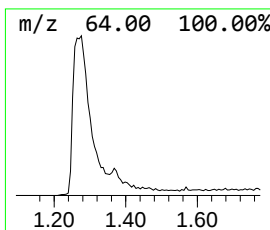
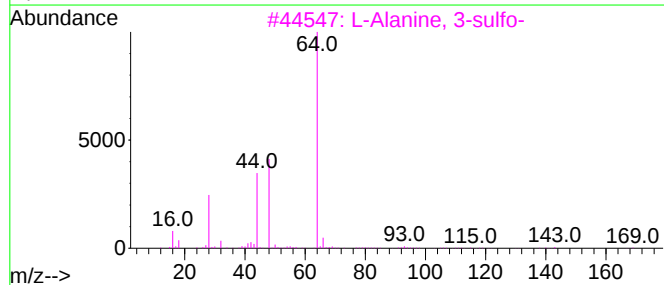
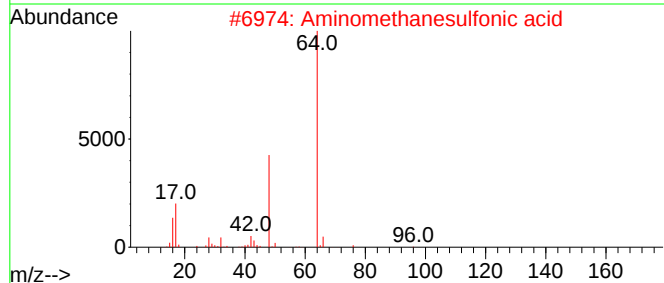
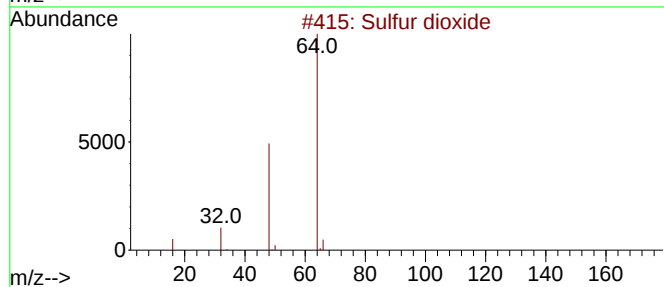
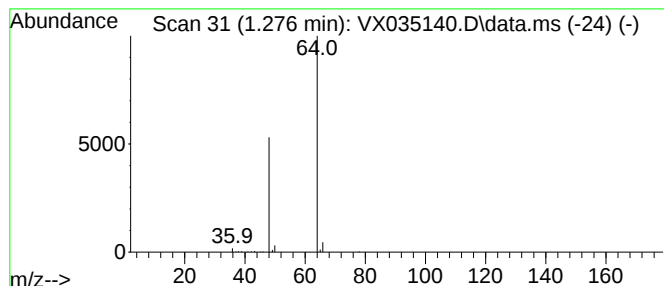
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.276	6.27 ug/L	144753	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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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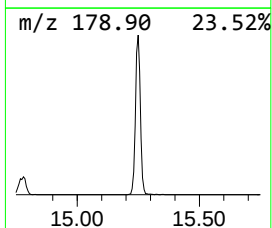
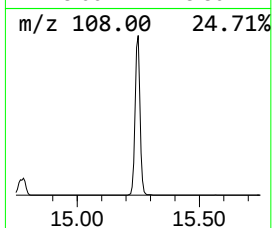
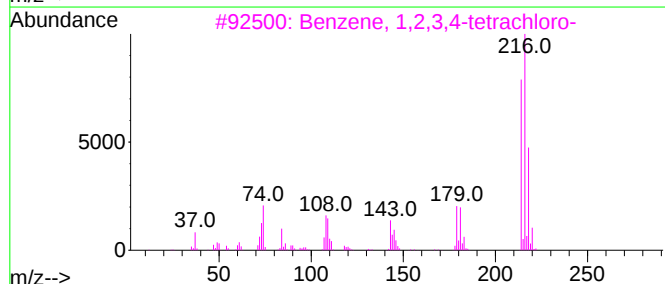
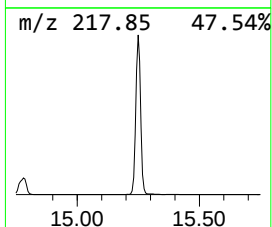
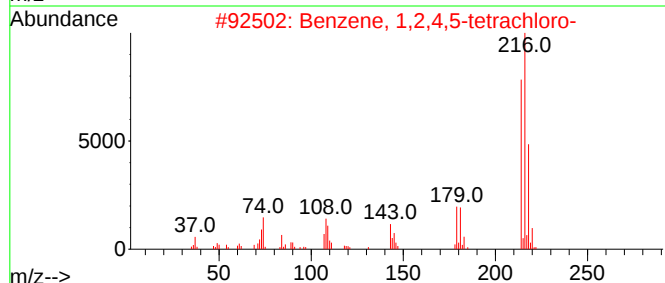
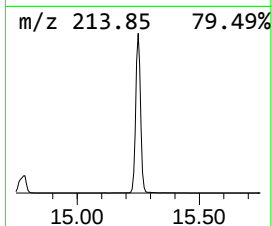
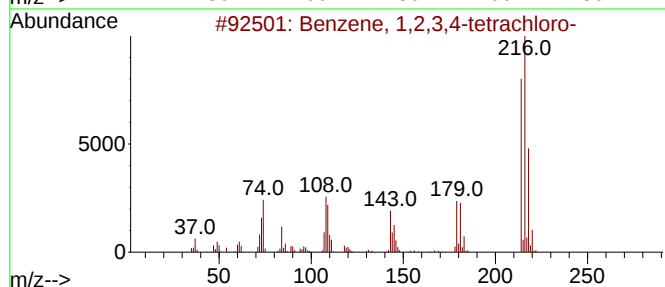
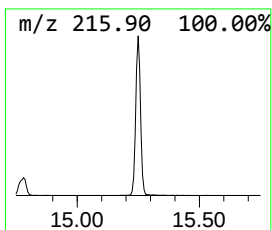
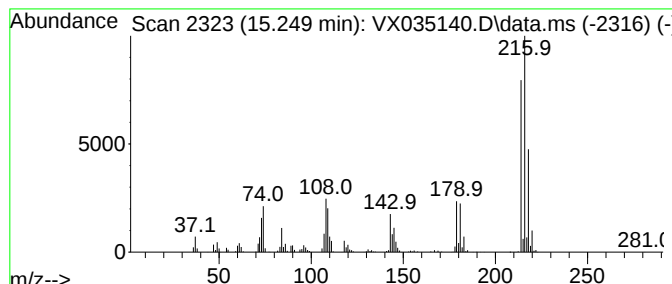
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Quant Title : VOC Analysis

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	9.02 ug/L	1125580	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, 1,2,3,5-tetrachloro-	214	C6H2Cl4	000634-90-2	99
5			Benzene, 1,2,3,5-tetrachloro-	214	C6H2Cl4	000634-90-2	98



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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
Sulfur dioxide	1.276	6.3	ug/L	144753	1	6.763	1153480	50.0
Benzene, 1,2,3,...	15.249	9.0	ug/L	1125580	3	12.024	6237500	50.0