

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035151.D
 Acq On : 19 Apr 2023 02:29
 Operator : JC/MD
 Sample : 02397-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 50 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM7

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: VX035151.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	6	9	18	rVB	27463	27202	1.31%	0.158%
2	1.258	24	28	42	rBV	74129	231470	11.19%	1.342%
3	1.368	43	46	54	rVB	270540	293840	14.20%	1.704%
4	1.673	92	96	106	rVB	179516	229847	11.11%	1.333%
5	2.307	194	200	210	rBV	446344	701685	33.91%	4.070%
6	2.861	289	291	292	rBV	383	199	0.01%	0.001%
7	2.935	300	303	310	rVB3	1071	1963	0.09%	0.011%
8	3.099	325	330	336	rVV6	1396	2529	0.12%	0.015%
9	3.447	382	387	393	rVB5	1262	2652	0.13%	0.015%
10	3.514	396	398	399	rVB2	289	207	0.01%	0.001%
11	3.532	399	401	404	rBV3	188	204	0.01%	0.001%
12	3.605	409	413	417	rVB3	449	772	0.04%	0.004%
13	3.666	420	423	426	rBV4	813	848	0.04%	0.005%
14	3.849	451	453	455	rVB2	240	182	0.01%	0.001%
15	3.873	455	457	460	rVB	258	219	0.01%	0.001%
16	3.898	460	461	464	rVB2	231	240	0.01%	0.001%
17	3.934	464	467	468	rBV2	515	527	0.03%	0.003%
18	4.172	500	506	509	rBV3	333	728	0.04%	0.004%
19	4.221	512	514	516	rBV2	409	330	0.02%	0.002%
20	4.264	519	521	525	rBV2	209	264	0.01%	0.002%
21	4.312	525	529	530	rBV2	389	349	0.02%	0.002%
22	4.459	542	553	575	rBV	120423	371868	17.97%	2.157%
23	4.910	624	627	629	rBV3	288	226	0.01%	0.001%
24	4.959	633	635	638	rBV2	169	199	0.01%	0.001%
25	5.056	638	651	673	rBV2	247676	775138	37.46%	4.496%
26	5.452	714	716	718	rBV3	189	214	0.01%	0.001%
27	5.477	718	720	723	rVB2	404	346	0.02%	0.002%
28	5.507	723	725	726	rBV	341	250	0.01%	0.001%
29	5.538	727	730	731	rBV	492	442	0.02%	0.003%
30	5.556	731	733	736	rVV2	950	919	0.04%	0.005%
31	5.654	746	749	750	rBV2	259	179	0.01%	0.001%
32	5.739	761	763	768	rVB3	263	395	0.02%	0.002%
33	5.775	768	769	771	rBV2	227	191	0.01%	0.001%
34	5.824	775	777	782	rVB2	382	561	0.03%	0.003%
35	5.873	782	785	787	rBV	151	217	0.01%	0.001%
36	5.971	788	801	808	rBV2	669481	2069457	100.00%	12.002%

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Integrator: RTE

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

37	6.221	840	842	843	rBV2	233	231	0.01%	0.001%
38	6.349	860	863	864	rBV	250	286	0.01%	0.002%
39	6.458	877	881	883	rBV3	268	316	0.02%	0.002%
40	6.556	895	897	901	rVB	368	308	0.01%	0.002%
41	6.629	908	909	911	rBV2	276	198	0.01%	0.001%
42	6.757	921	930	951	rBV	433383	1048731	50.68%	6.082%
43	7.056	976	979	984	rBV3	436	800	0.04%	0.005%
44	7.117	984	989	996	rVV4	1854	4121	0.20%	0.024%
45	7.178	997	999	1000	rVB	329	185	0.01%	0.001%
46	7.306	1011	1020	1042	rBV	410488	910810	44.01%	5.282%
47	7.793	1098	1100	1104	rVB2	244	307	0.01%	0.002%
48	7.946	1120	1125	1132	rVV4	1576	2974	0.14%	0.017%
49	8.043	1137	1141	1142	rVB	478	398	0.02%	0.002%
50	8.226	1169	1171	1175	rBV2	279	416	0.02%	0.002%
51	8.324	1181	1187	1205	rBV	252965	422033	20.39%	2.448%
52	8.647	1233	1240	1252	rBV	1078787	1662680	80.34%	9.643%
53	8.811	1265	1267	1270	rBV3	535	357	0.02%	0.002%
54	8.952	1284	1290	1304	rBV	171757	264862	12.80%	1.536%
55	9.165	1322	1325	1328	rBV3	385	664	0.03%	0.004%
56	9.269	1339	1342	1353	rVB4	1395	1942	0.09%	0.011%
57	9.385	1355	1361	1377	rBV	571199	819884	39.62%	4.755%
58	9.592	1394	1395	1401	rVV3	534	645	0.03%	0.004%
59	9.635	1401	1402	1403	rVB	553	202	0.01%	0.001%
60	9.726	1414	1417	1419	rBV3	486	672	0.03%	0.004%
61	9.945	1451	1453	1456	rVV2	371	312	0.02%	0.002%
62	10.055	1465	1471	1473	rBV	890604	1399131	67.61%	8.115%
63	10.427	1527	1532	1537	rBV4	524	793	0.04%	0.005%
64	10.494	1542	1543	1545	rBV2	293	217	0.01%	0.001%
65	10.640	1564	1567	1570	rBV3	346	553	0.03%	0.003%
66	10.842	1598	1600	1602	rBV	240	198	0.01%	0.001%
67	10.866	1602	1604	1605	rBV	291	239	0.01%	0.001%
68	10.945	1615	1617	1622	rVB2	405	571	0.03%	0.003%
69	10.994	1622	1625	1626	rBV	287	209	0.01%	0.001%
70	11.189	1652	1657	1668	rBV	670433	869202	42.00%	5.041%
71	11.311	1674	1677	1681	rVB3	689	845	0.04%	0.005%
72	11.402	1687	1692	1694	rVB2	465	476	0.02%	0.003%
73	11.512	1707	1710	1713	rBV2	439	552	0.03%	0.003%
74	11.549	1713	1716	1717	rBV2	204	194	0.01%	0.001%
75	11.707	1739	1742	1746	rVB3	924	1043	0.05%	0.006%
76	11.744	1746	1748	1750	rBV2	266	234	0.01%	0.001%

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Sampling : 1

Min Area: 0 % of largest Peak

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Peak Location: TOP

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 Title : VOC Analysis

77	11.762	1750	1751	1753	rVB2	399	182	0.01%	0.001%
78	11.848	1763	1765	1767	rBV2	535	458	0.02%	0.003%
79	11.902	1772	1774	1776	rVB2	280	208	0.01%	0.001%
80	11.969	1779	1785	1789	rBV	60579	76441	3.69%	0.443%
81	12.024	1789	1794	1805	rVB2	901687	1717330	82.98%	9.960%
82	12.226	1823	1827	1832	rBV4	3670	6218	0.30%	0.036%
83	12.323	1837	1843	1852	rVV3	1117079	1891072	91.38%	10.968%
84	12.841	1926	1928	1929	rBV	400	299	0.01%	0.002%
85	12.927	1938	1942	1948	rVB2	2669	3711	0.18%	0.022%
86	13.061	1959	1964	1969	rBV4	3494	6223	0.30%	0.036%
87	13.110	1969	1972	1978	rVV3	2671	3740	0.18%	0.022%
88	13.164	1978	1981	1982	rVV2	290	255	0.01%	0.001%
89	13.195	1982	1986	1990	rVB4	1759	2517	0.12%	0.015%
90	13.359	2011	2013	2014	rBV2	346	246	0.01%	0.001%
91	13.530	2039	2041	2042	rBV2	350	277	0.01%	0.002%
92	13.585	2043	2050	2069	rVB	807485	1010485	48.83%	5.861%
93	13.872	2096	2097	2098	rBV	536	293	0.01%	0.002%
94	13.963	2105	2112	2123	rBV	195465	257555	12.45%	1.494%
95	14.506	2199	2201	2204	rBV3	344	442	0.02%	0.003%
96	14.542	2205	2207	2209	rVB2	478	309	0.01%	0.002%
97	14.621	2219	2220	2222	rBV	531	360	0.02%	0.002%
98	14.786	2240	2247	2252	rBV	20179	32710	1.58%	0.190%
99	15.249	2317	2323	2330	rBV	66196	93845	4.53%	0.544%
100	16.383	2505	2509	2511	rBV3	813	1424	0.07%	0.008%

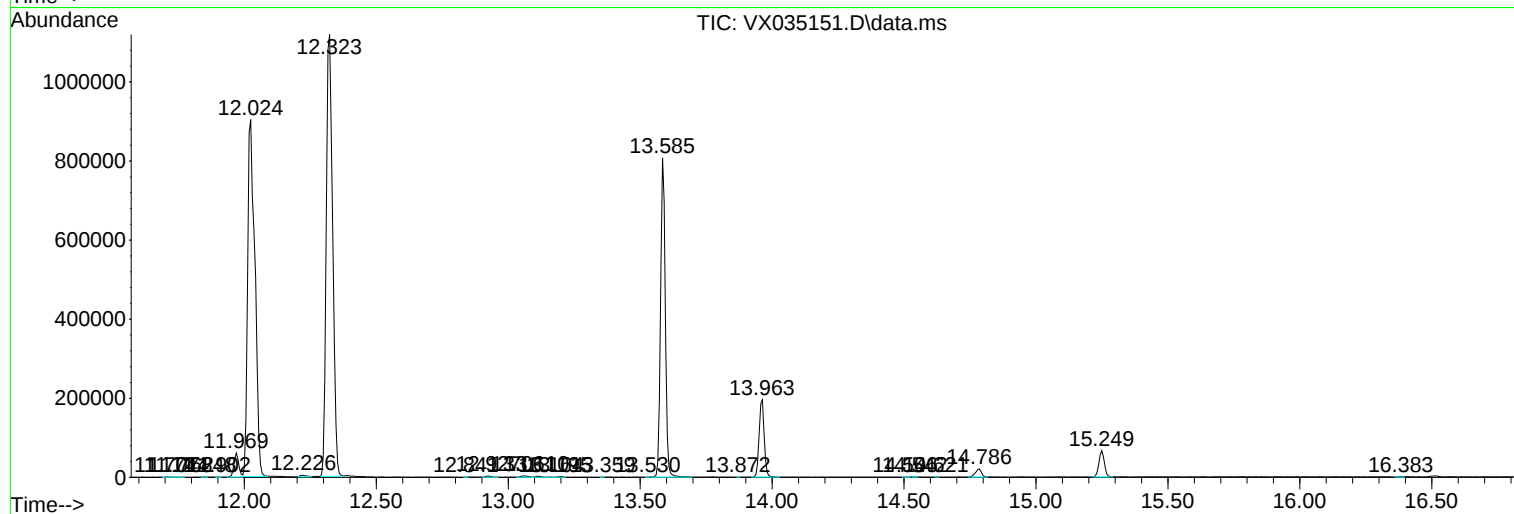
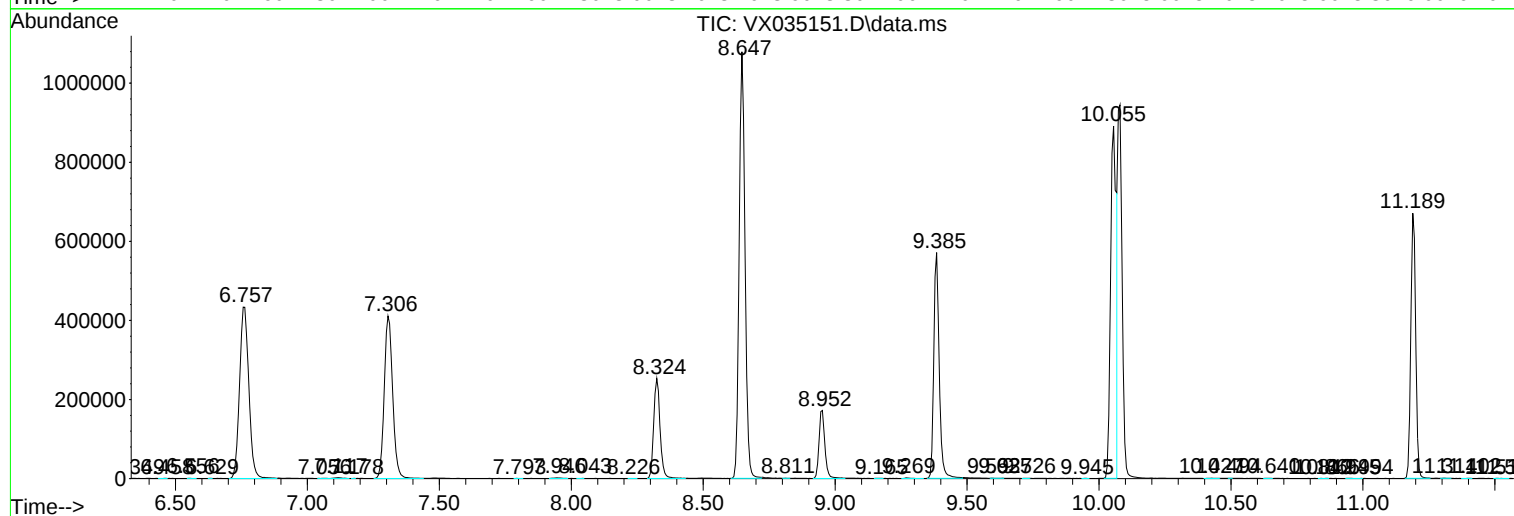
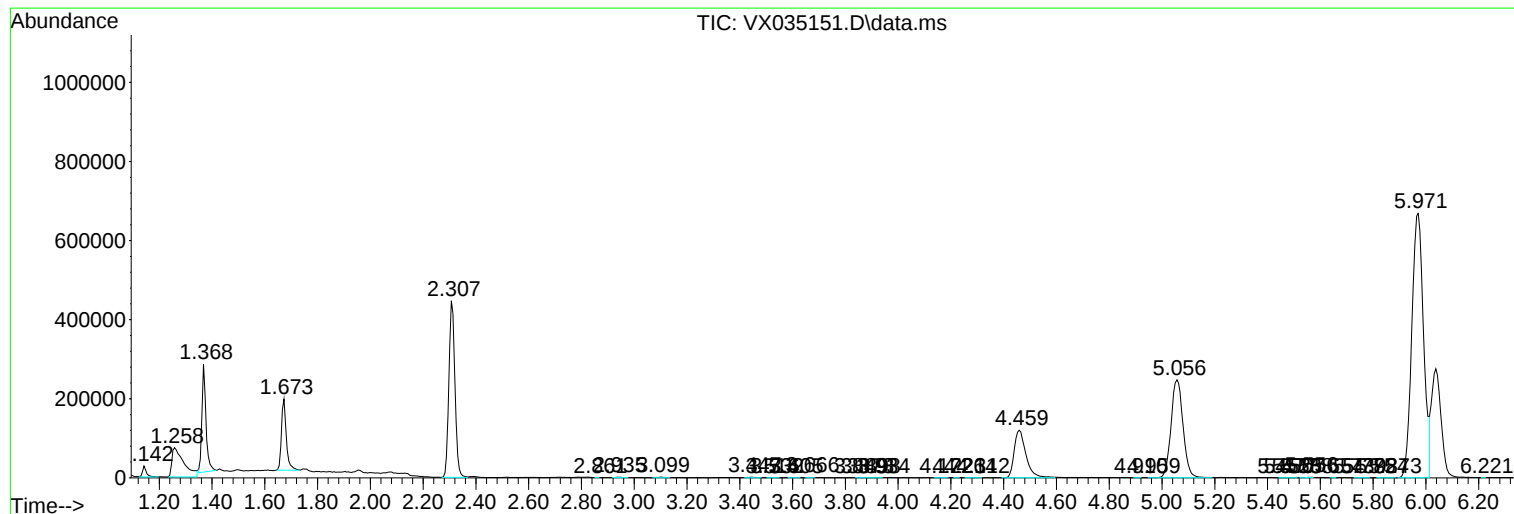
Sum of corrected areas: 17242250

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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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO41823\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

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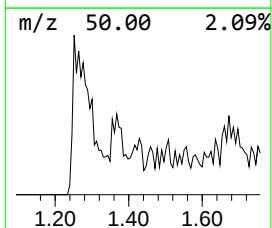
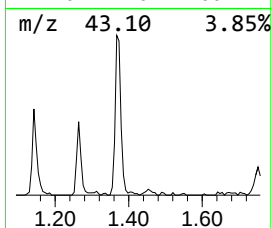
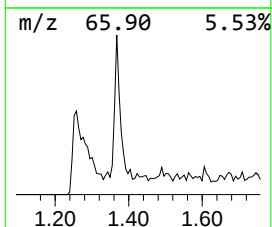
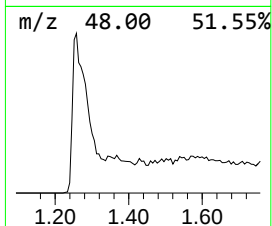
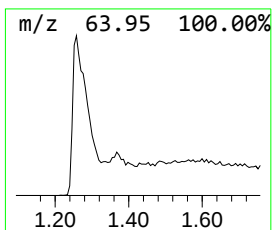
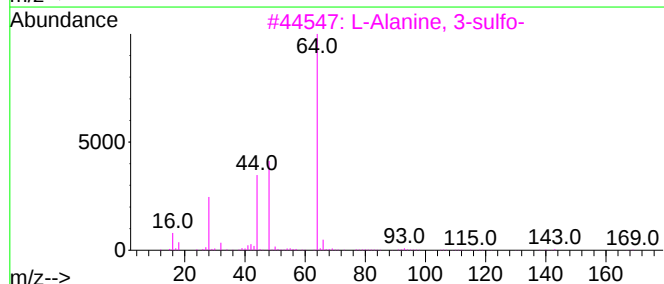
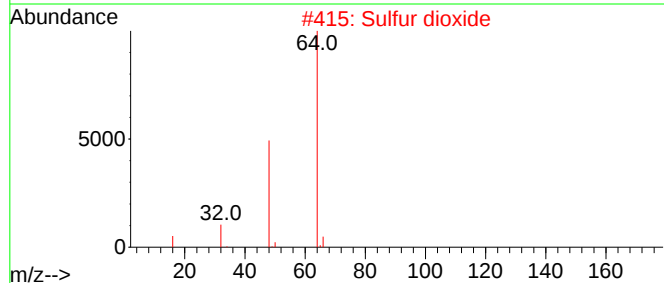
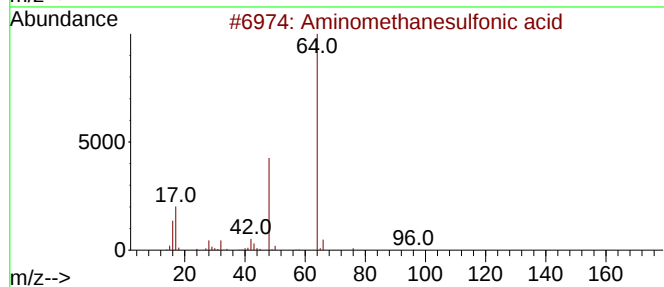
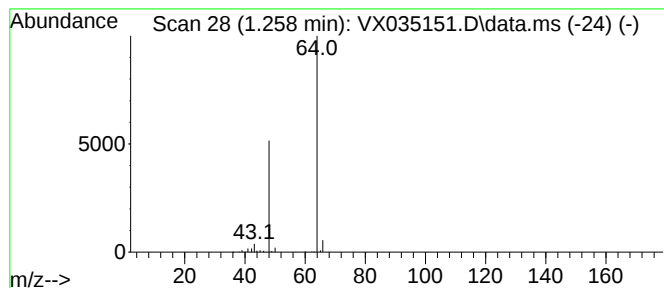
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	11.04 ug/L	231470	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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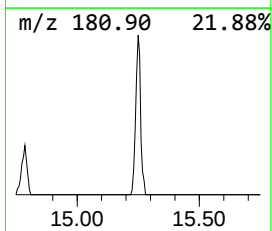
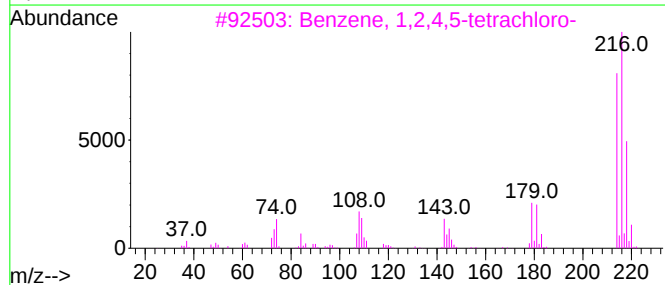
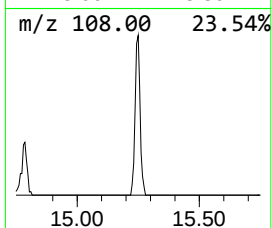
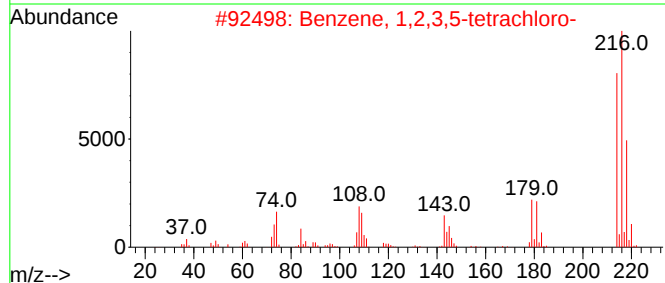
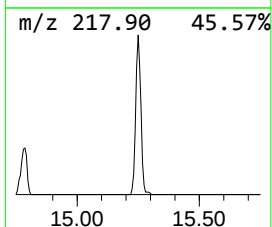
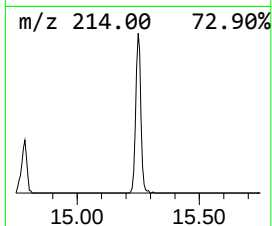
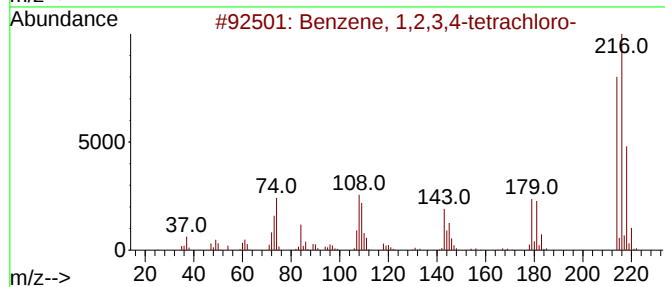
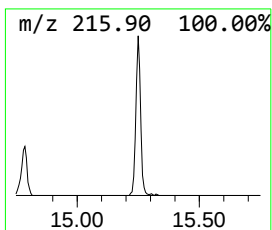
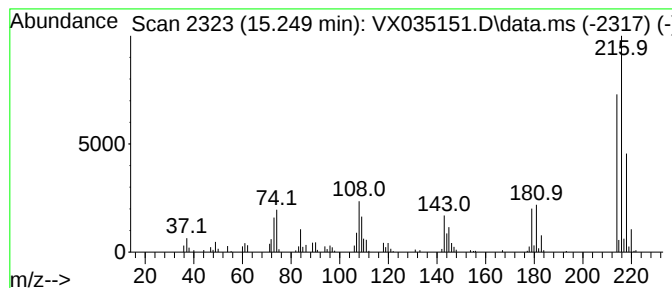
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Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.249	2.73 ug/L	93845	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, 1,2,3,5-tetrachloro-	214	C6H2Cl4	000634-90-2	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	98
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
Aminomethanesul...	1.258	11.0	ug/L	231470	1	6.763	1048730	50.0
Benzene, 1,2,3,...	15.249	2.7	ug/L	93845	3	12.024	1717330	50.0