

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042779.D
 Acq On : 31 Jul 2024 17:34
 Operator : JC/MD
 Sample : P3398-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08K6

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042779.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	rVB2	1527	1978	0.34%	0.047%
2	1.240	22	25	33	rBV	14377	20723	3.51%	0.497%
3	1.368	43	46	58	rBV	32236	43322	7.34%	1.039%
4	1.453	58	60	65	rVB	1356	1589	0.27%	0.038%
5	1.496	65	67	69	rBV2	305	371	0.06%	0.009%
6	1.563	74	78	79	rBV3	1152	1645	0.28%	0.039%
7	1.648	89	92	102	rVB	25509	29841	5.06%	0.716%
8	1.886	130	131	133	rBV	219	192	0.03%	0.005%
9	2.294	192	198	209	rBV	88336	138332	23.45%	3.317%
10	2.386	211	213	221	rVB4	1687	2850	0.48%	0.068%
11	2.508	230	233	236	rBV	303	315	0.05%	0.008%
12	2.556	239	241	242	rVV	235	210	0.04%	0.005%
13	2.575	242	244	246	rVB2	393	229	0.04%	0.005%
14	2.788	274	279	285	rVV3	908	1671	0.28%	0.040%
15	2.940	298	304	313	rBV2	1883	4336	0.74%	0.104%
16	3.142	332	337	340	rBV	188	370	0.06%	0.009%
17	3.270	356	358	361	rBV	194	244	0.04%	0.006%
18	3.446	384	387	390	rBV	253	298	0.05%	0.007%
19	3.623	414	416	418	rVV	221	242	0.04%	0.006%
20	3.751	434	437	438	rBV	161	193	0.03%	0.005%
21	3.861	452	455	458	rBV2	166	254	0.04%	0.006%
22	3.983	472	475	480	rBV	175	339	0.06%	0.008%
23	4.123	493	498	500	rVB	245	385	0.07%	0.009%
24	4.148	500	502	506	rBV2	243	386	0.07%	0.009%
25	4.196	506	510	513	rVB	236	302	0.05%	0.007%
26	4.282	520	524	527	rBV	242	318	0.05%	0.008%
27	4.306	527	528	531	rBV	266	203	0.03%	0.005%
28	4.410	541	545	546	rBV	334	341	0.06%	0.008%
29	4.471	547	555	571	rBV	33543	99814	16.92%	2.393%
30	4.800	607	609	613	rVB	271	315	0.05%	0.008%
31	4.849	616	617	621	rVB	248	218	0.04%	0.005%
32	4.964	633	636	638	rBV	163	195	0.03%	0.005%
33	5.056	640	651	669	rBV2	69128	215625	36.55%	5.171%
34	5.221	676	678	681	rBV2	253	242	0.04%	0.006%
35	5.385	703	705	706	rBV	283	223	0.04%	0.005%
36	5.495	722	723	725	rBV	246	212	0.04%	0.005%

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 Title : VOC Analysis

37	5.562	730	734	735	rBV3	448	531	0.09%	0.013%
38	5.806	772	774	776	rBV2	175	186	0.03%	0.004%
39	5.964	789	800	820	rBV3	200395	589925	100.00%	14.146%
40	6.184	834	836	838	rBV	296	195	0.03%	0.005%
41	6.385	867	869	871	rVB	441	334	0.06%	0.008%
42	6.403	871	872	875	rBV2	252	290	0.05%	0.007%
43	6.763	922	931	950	rBV	145649	355642	60.29%	8.528%
44	7.117	986	989	994	rVB4	884	1212	0.21%	0.029%
45	7.226	1004	1007	1010	rBV2	390	517	0.09%	0.012%
46	7.312	1012	1021	1035	rBV	117355	264259	44.80%	6.337%
47	7.488	1046	1050	1054	rVB3	378	523	0.09%	0.013%
48	7.537	1056	1058	1063	rVB2	340	322	0.05%	0.008%
49	7.824	1100	1105	1112	rBV3	2887	5907	1.00%	0.142%
50	8.330	1182	1188	1199	rBV2	66855	117824	19.97%	2.825%
51	8.580	1226	1229	1233	rVB3	492	722	0.12%	0.017%
52	8.647	1233	1240	1256	rBV	273489	445155	75.46%	10.674%
53	8.952	1285	1290	1307	rBV	47635	73984	12.54%	1.774%
54	9.098	1313	1314	1316	rBV	277	231	0.04%	0.006%
55	9.275	1338	1343	1349	rVB	3178	4632	0.79%	0.111%
56	9.391	1356	1362	1370	rBV	183703	281161	47.66%	6.742%
57	9.531	1380	1385	1393	rVB4	6917	13442	2.28%	0.322%
58	9.653	1402	1405	1407	rBV2	304	264	0.04%	0.006%
59	9.903	1442	1446	1447	rBV2	268	250	0.04%	0.006%
60	10.055	1465	1471	1489	rBV	297250	413808	70.15%	9.923%
61	10.201	1492	1495	1497	rBV2	451	426	0.07%	0.010%
62	10.451	1532	1536	1537	rBV	213	302	0.05%	0.007%
63	10.512	1544	1546	1551	rBV2	258	404	0.07%	0.010%
64	10.720	1578	1580	1582	rVB	299	205	0.03%	0.005%
65	10.805	1590	1594	1598	rBV3	2622	3551	0.60%	0.085%
66	10.878	1601	1606	1611	rBV2	569	787	0.13%	0.019%
67	10.957	1618	1619	1623	rVB2	325	361	0.06%	0.009%
68	11.104	1641	1643	1646	rBV	217	200	0.03%	0.005%
69	11.146	1649	1650	1652	rBV	254	216	0.04%	0.005%
70	11.195	1652	1658	1667	rVV	222165	294494	49.92%	7.062%
71	11.311	1674	1677	1682	rVB2	2413	3111	0.53%	0.075%
72	11.415	1692	1694	1696	rBV2	189	196	0.03%	0.005%
73	11.841	1762	1764	1768	rBV2	199	246	0.04%	0.006%
74	11.933	1776	1779	1783	rVB2	1333	1366	0.23%	0.033%
75	12.024	1789	1794	1807	rVB	261971	340310	57.69%	8.160%
76	12.140	1812	1813	1815	rVB	362	195	0.03%	0.005%

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 Title : VOC Analysis

77	12.225	1823	1827	1833	rVB5	801	1687	0.29%	0.040%
78	12.317	1837	1842	1854	rBV	270013	357065	60.53%	8.562%
79	12.530	1876	1877	1879	rBV	263	191	0.03%	0.005%
80	12.579	1879	1885	1886	rBV2	205	370	0.06%	0.009%
81	12.701	1903	1905	1907	rBV2	275	236	0.04%	0.006%
82	12.756	1911	1914	1919	rBV2	836	905	0.15%	0.022%
83	12.805	1920	1922	1924	rBV	355	231	0.04%	0.006%
84	12.865	1928	1932	1936	rBV4	1835	2557	0.43%	0.061%
85	13.426	2021	2024	2025	rBV2	331	272	0.05%	0.007%
86	13.487	2031	2034	2035	rBV	285	213	0.04%	0.005%
87	13.646	2059	2060	2063	rVB	395	308	0.05%	0.007%
88	13.774	2077	2081	2094	rBV	7077	11744	1.99%	0.282%
89	13.878	2097	2098	2101	rVB2	530	425	0.07%	0.010%
90	14.134	2136	2140	2142	rVB2	1693	2089	0.35%	0.050%
91	14.481	2195	2197	2199	rBV2	350	401	0.07%	0.010%
92	14.579	2211	2213	2216	rBV	327	276	0.05%	0.007%
93	14.646	2222	2224	2228	rVB2	817	765	0.13%	0.018%
94	14.713	2233	2235	2238	rVV2	219	240	0.04%	0.006%
95	14.835	2251	2255	2257	rVB2	307	396	0.07%	0.009%
96	15.060	2290	2292	2294	rBV2	293	270	0.05%	0.006%
97	15.097	2297	2298	2300	rBV	327	215	0.04%	0.005%
98	15.396	2342	2347	2351	rVB2	1695	2930	0.50%	0.070%
99	16.176	2474	2475	2477	rBV	431	229	0.04%	0.005%
100	16.755	2569	2570	2572	rVB2	518	268	0.05%	0.006%

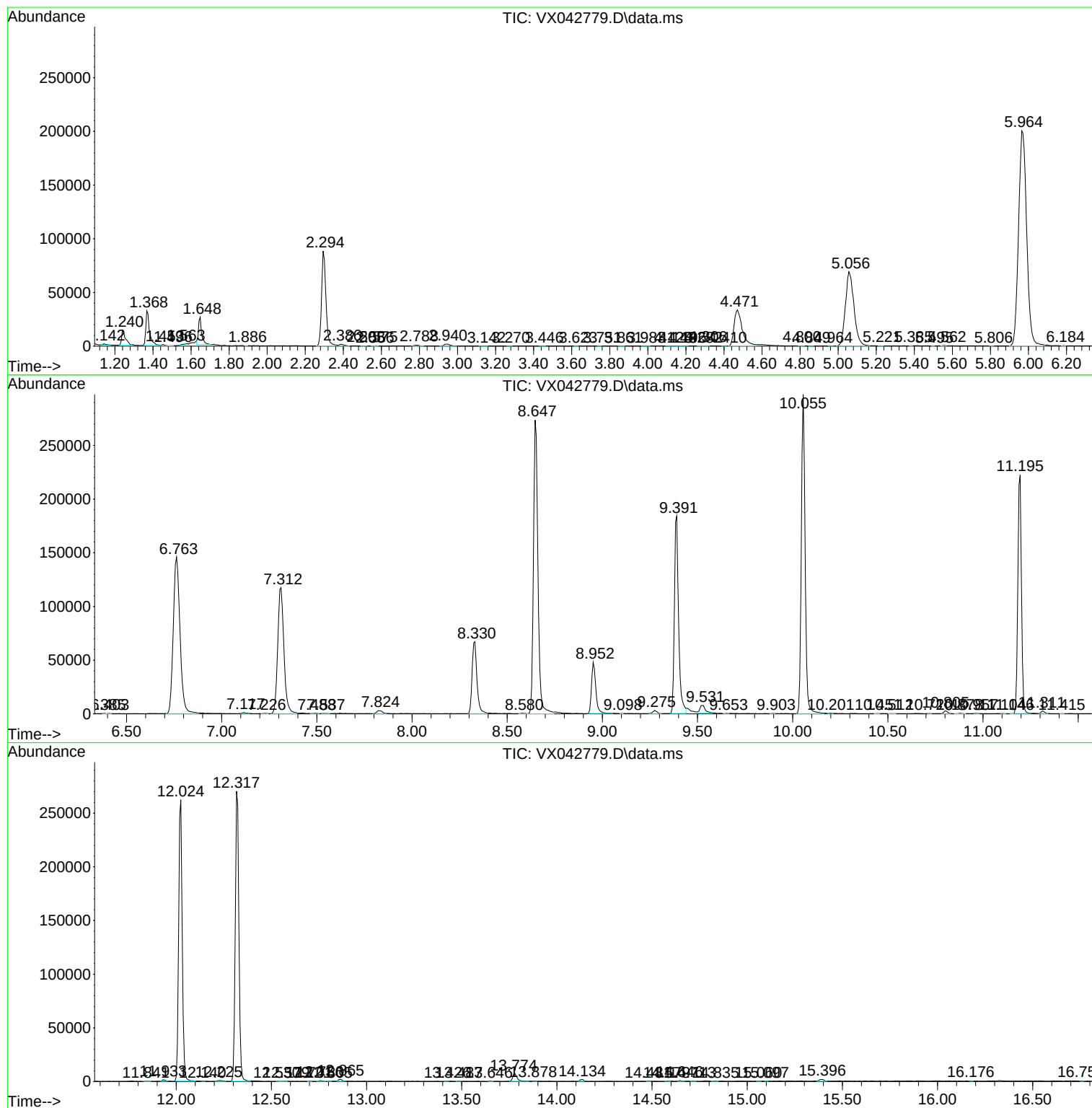
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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



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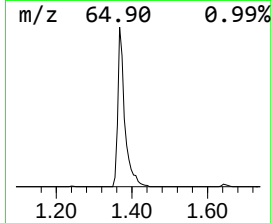
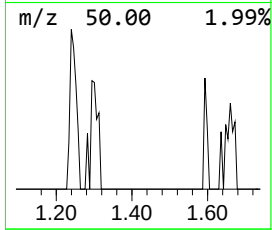
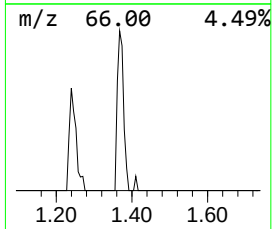
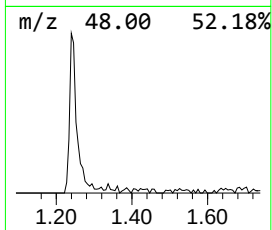
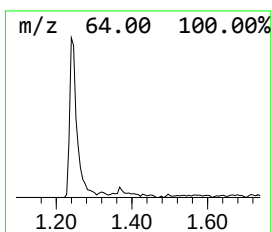
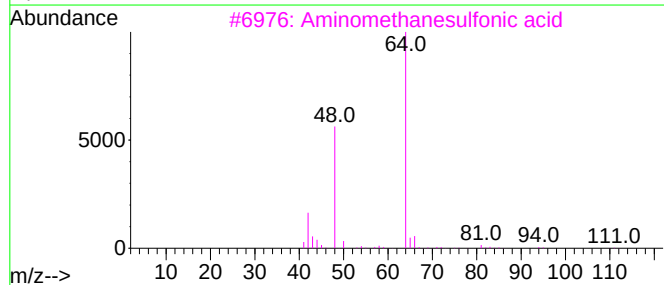
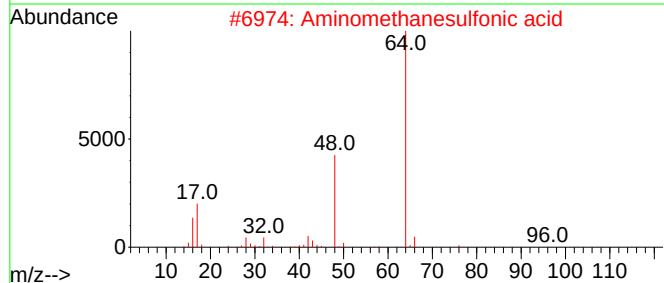
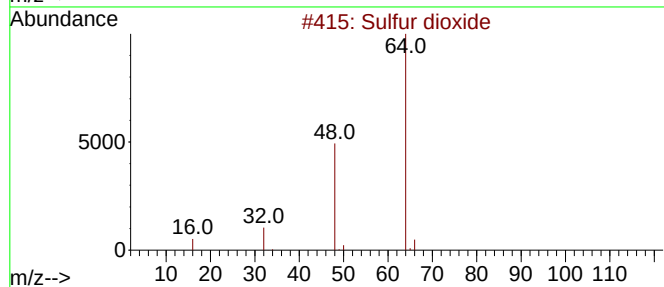
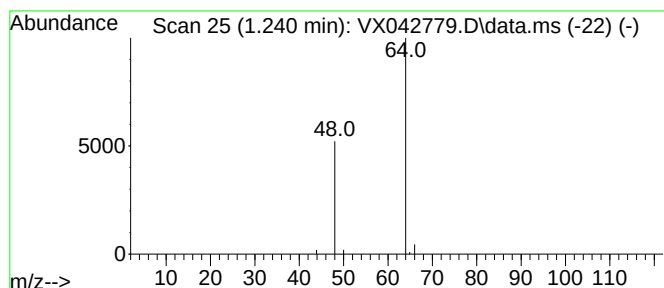
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
1.240	2.91 ug/L	20723	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	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	2.9	ug/L	20723	1	6.763	355642	50.0