

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042777.D
 Acq On : 31 Jul 2024 16:47
 Operator : JC/MD
 Sample : P3398-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L7

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: VX042777.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	32	rBV2	13266	19074	3.44%	0.483%
2	1.367	43	46	57	rVB	35953	45542	8.21%	1.152%
3	1.507	67	69	71	rBV2	264	316	0.06%	0.008%
4	1.556	72	77	78	rBV3	1034	1477	0.27%	0.037%
5	1.581	78	81	83	rBV3	1543	2660	0.48%	0.067%
6	1.648	88	92	101	rVB	27266	35112	6.33%	0.888%
7	1.788	113	115	117	rBV	579	540	0.10%	0.014%
8	1.837	121	123	124	rVB	552	345	0.06%	0.009%
9	1.995	148	149	153	rBV2	277	299	0.05%	0.008%
10	2.141	170	173	175	rBV	265	284	0.05%	0.007%
11	2.294	192	198	209	rBV	83915	135438	24.40%	3.426%
12	2.458	222	225	228	rBB2	269	261	0.05%	0.007%
13	2.568	242	243	248	rBV	312	377	0.07%	0.010%
14	2.794	275	280	282	rVV2	809	1132	0.20%	0.029%
15	2.946	298	305	311	rBV	1817	3920	0.71%	0.099%
16	3.074	324	326	327	rBV	317	268	0.05%	0.007%
17	3.385	372	377	379	rBV2	178	313	0.06%	0.008%
18	3.696	425	428	432	rBB	217	260	0.05%	0.007%
19	4.293	524	526	531	rVB	218	368	0.07%	0.009%
20	4.385	538	541	544	rBV	189	284	0.05%	0.007%
21	4.470	547	555	567	rBV2	31490	92508	16.67%	2.340%
22	4.836	613	615	617	rBV	326	285	0.05%	0.007%
23	4.915	623	628	630	rBV2	236	361	0.07%	0.009%
24	5.056	639	651	667	rBV	63091	194869	35.11%	4.930%
25	5.202	674	675	678	rVB	329	238	0.04%	0.006%
26	5.226	678	679	683	rBV	222	278	0.05%	0.007%
27	5.269	683	686	688	rBV	211	218	0.04%	0.006%
28	5.354	697	700	704	rVB2	269	317	0.06%	0.008%
29	5.391	704	706	707	rBV	446	355	0.06%	0.009%
30	5.531	727	729	731	rBV	277	239	0.04%	0.006%
31	5.641	745	747	750	rVB	349	299	0.05%	0.008%
32	5.677	751	753	755	rBV	250	227	0.04%	0.006%
33	5.866	782	784	786	rBV	259	283	0.05%	0.007%
34	5.970	790	801	817	rBV2	190960	555045	100.00%	14.041%
35	6.110	822	824	827	rVB2	538	476	0.09%	0.012%
36	6.311	855	857	860	rVB	324	276	0.05%	0.007%

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

37	6.604	904	905	911	rVB2	202	290	0.05%	0.007%
38	6.763	922	931	946	rBV	139376	333460	60.08%	8.436%
39	6.976	964	966	968	rVB	383	284	0.05%	0.007%
40	7.080	981	983	985	rVB2	379	296	0.05%	0.007%
41	7.110	985	988	989	rBV2	905	890	0.16%	0.023%
42	7.220	1003	1006	1009	rVB	374	315	0.06%	0.008%
43	7.311	1013	1021	1038	rBV	110045	246933	44.49%	6.247%
44	7.518	1053	1055	1058	rVB	309	273	0.05%	0.007%
45	7.762	1092	1095	1097	rBV	336	393	0.07%	0.010%
46	7.909	1117	1119	1124	rVB2	326	371	0.07%	0.009%
47	7.964	1124	1128	1130	rBV	304	365	0.07%	0.009%
48	8.110	1150	1152	1153	rBV	244	236	0.04%	0.006%
49	8.323	1182	1187	1204	rBV	63975	111625	20.11%	2.824%
50	8.646	1234	1240	1250	rBV	258316	425468	76.65%	10.763%
51	8.951	1285	1290	1301	rBV	46734	71628	12.90%	1.812%
52	9.061	1306	1308	1311	rBV2	345	398	0.07%	0.010%
53	9.274	1337	1343	1352	rBV2	2526	4353	0.78%	0.110%
54	9.341	1352	1354	1356	rBV	232	281	0.05%	0.007%
55	9.390	1356	1362	1377	rBV	167784	263253	47.43%	6.660%
56	9.585	1393	1394	1395	rVB	628	230	0.04%	0.006%
57	9.957	1453	1455	1458	rVB2	238	253	0.05%	0.006%
58	10.000	1458	1462	1463	rBV	234	273	0.05%	0.007%
59	10.055	1465	1471	1487	rBV	270836	383375	69.07%	9.698%
60	10.201	1493	1495	1501	rVB5	751	1100	0.20%	0.028%
61	10.274	1504	1507	1510	rBV2	273	477	0.09%	0.012%
62	10.311	1510	1513	1518	rVB2	1215	1656	0.30%	0.042%
63	10.463	1537	1538	1544	rVB2	257	398	0.07%	0.010%
64	10.524	1544	1548	1550	rBV2	199	252	0.05%	0.006%
65	10.597	1557	1560	1561	rVV2	246	261	0.05%	0.007%
66	10.646	1564	1568	1575	rBV2	791	1315	0.24%	0.033%
67	10.786	1590	1591	1595	rBV2	242	311	0.06%	0.008%
68	10.829	1595	1598	1600	rVB2	210	248	0.04%	0.006%
69	11.036	1629	1632	1636	rBV2	562	654	0.12%	0.017%
70	11.195	1652	1658	1666	rBV	215793	282108	50.83%	7.137%
71	11.310	1672	1677	1682	rBV4	2422	2977	0.54%	0.075%
72	11.756	1747	1750	1754	rVB2	523	610	0.11%	0.015%
73	12.024	1789	1794	1806	rBV	259451	323144	58.22%	8.175%
74	12.237	1825	1829	1834	rBV6	1098	1433	0.26%	0.036%
75	12.316	1837	1842	1853	rBV	272169	362818	65.37%	9.178%
76	12.463	1864	1866	1867	rBV	314	228	0.04%	0.006%

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 Title : VOC Analysis

77	12.554	1879	1881	1884	rBV2	210	228	0.04%	0.006%
78	12.774	1911	1917	1920	rVB4	567	932	0.17%	0.024%
79	12.804	1920	1922	1925	rBV2	317	393	0.07%	0.010%
80	13.097	1968	1970	1973	rBV2	237	237	0.04%	0.006%
81	13.627	2055	2057	2061	rVB	295	319	0.06%	0.008%
82	13.664	2061	2063	2065	rBV	197	235	0.04%	0.006%
83	13.780	2077	2082	2090	rVV	11200	15952	2.87%	0.404%
84	13.877	2093	2098	2104	rVB2	697	1480	0.27%	0.037%
85	14.127	2136	2139	2143	rVB	1815	1844	0.33%	0.047%
86	14.444	2188	2191	2193	rVV2	334	438	0.08%	0.011%
87	14.462	2193	2194	2198	rVV	477	519	0.09%	0.013%
88	14.493	2198	2199	2201	rVV2	407	330	0.06%	0.008%
89	14.548	2205	2208	2211	rBV3	393	563	0.10%	0.014%
90	14.584	2212	2214	2218	rVV2	547	585	0.11%	0.015%
91	14.645	2221	2224	2229	rVB4	785	1269	0.23%	0.032%
92	14.785	2244	2247	2250	rVB3	842	1197	0.22%	0.030%
93	15.090	2296	2297	2300	rBV	412	406	0.07%	0.010%
94	15.389	2343	2346	2351	rVB3	1607	2282	0.41%	0.058%
95	15.487	2361	2362	2365	rBV2	380	337	0.06%	0.009%
96	15.865	2422	2424	2426	rBV2	348	343	0.06%	0.009%
97	15.993	2443	2445	2449	rVB3	414	518	0.09%	0.013%
98	16.029	2449	2451	2454	rBV2	337	303	0.05%	0.008%
99	16.328	2497	2500	2503	rBV3	785	1205	0.22%	0.030%
100	16.700	2556	2561	2562	rBV2	908	1279	0.23%	0.032%

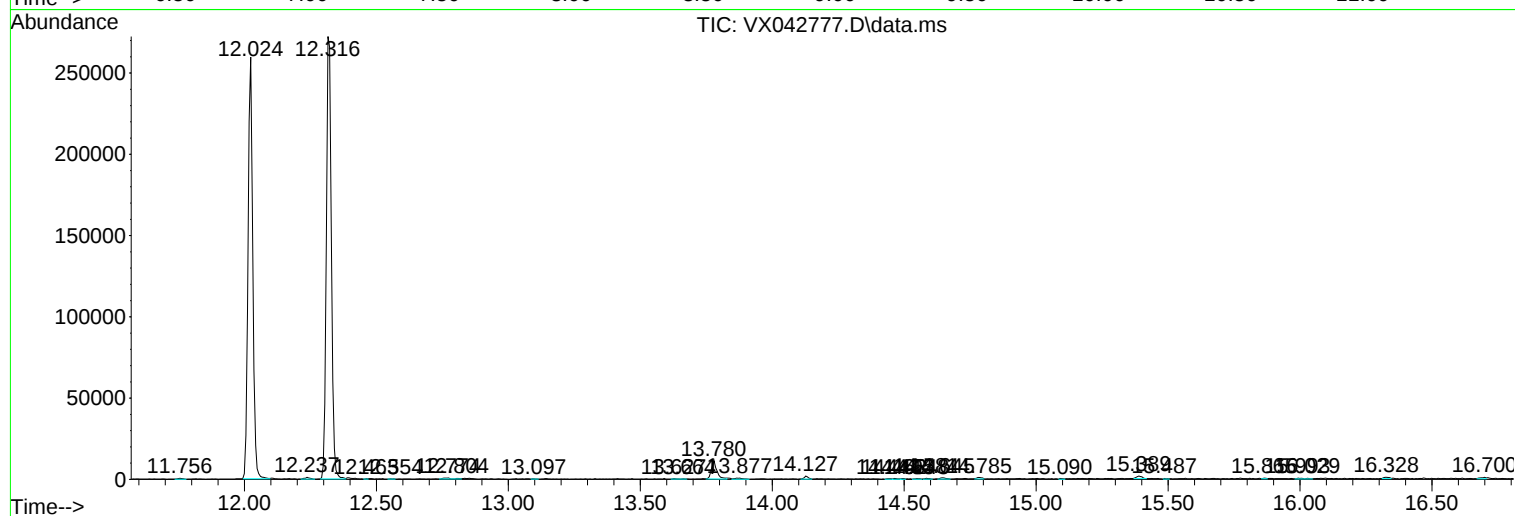
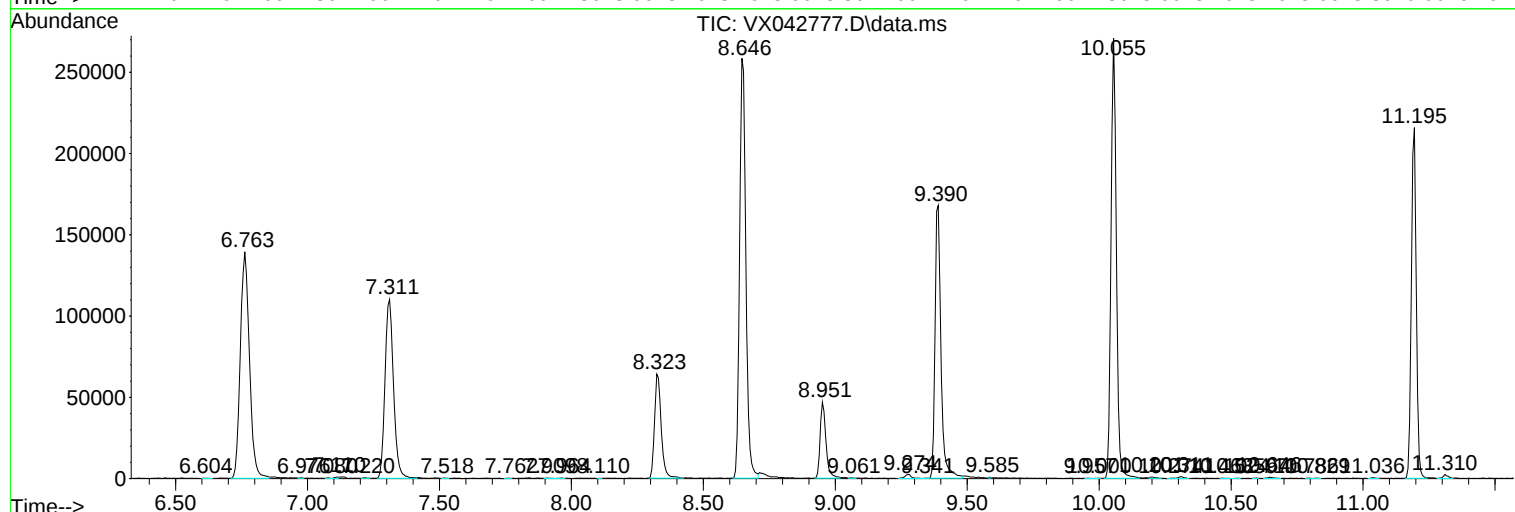
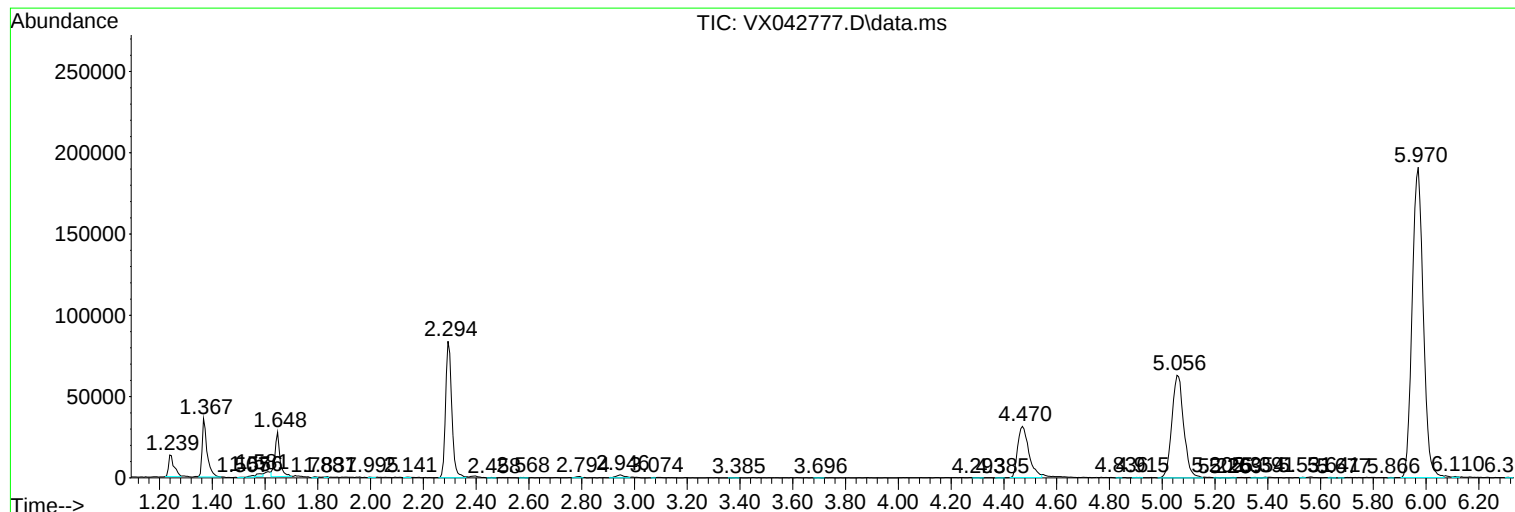
Sum of corrected areas: 3952971

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Instrument :
MSVOA_X
ClientSampleId :
E08L7

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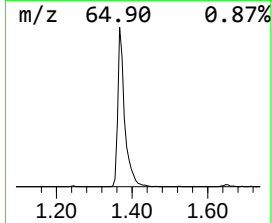
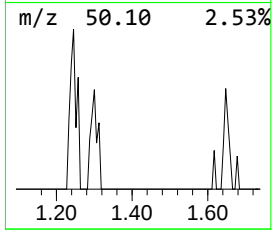
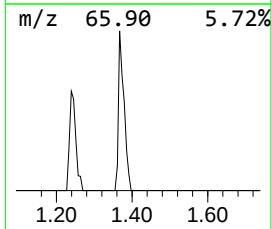
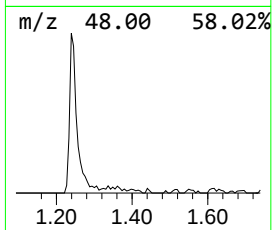
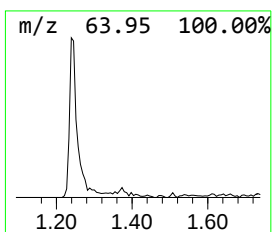
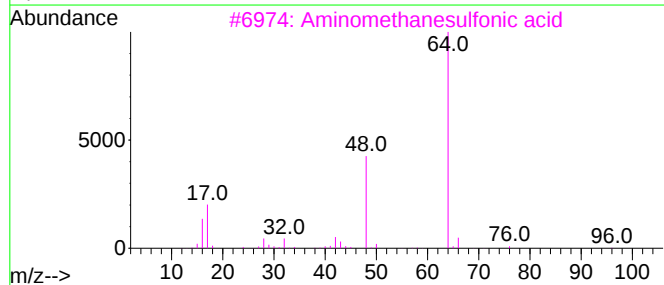
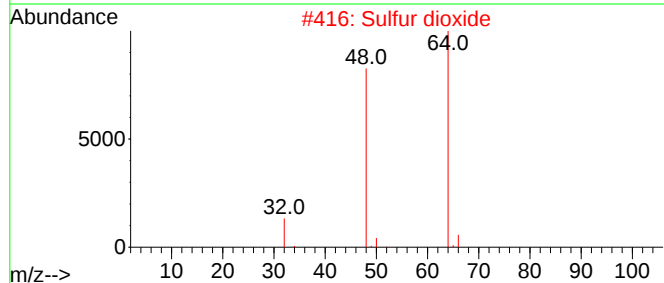
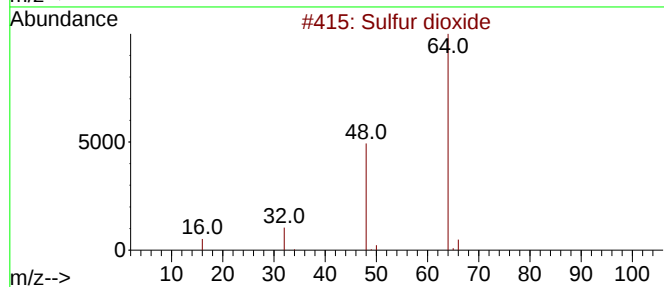
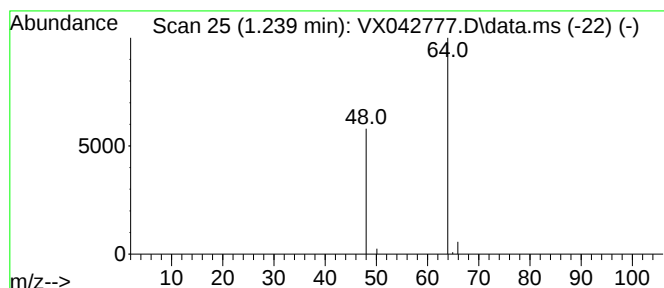
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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.
1.239	2.86 ug/L	19074	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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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	1.239	2.9	ug/L	19074	1	6.763	333460	50.0