

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042480.D
 Acq On : 23 Jul 2024 18:27
 Operator : JC/MD
 Sample : P3327-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZW6

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042480.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	17	rVB2	5619	7200	1.14%	0.149%
2	1.240	22	25	28	rBV	33894	35843	5.67%	0.743%
3	1.368	43	46	58	rVB	82361	103730	16.41%	2.150%
4	1.648	88	92	101	rVB	48134	63748	10.09%	1.321%
5	2.294	192	198	209	rBV	130884	206292	32.64%	4.275%
6	2.502	229	232	236	rVV2	339	464	0.07%	0.010%
7	2.569	239	243	249	rBV2	381	689	0.11%	0.014%
8	2.788	273	279	281	rBV4	822	1561	0.25%	0.032%
9	2.947	299	305	314	rBV2	2529	6010	0.95%	0.125%
10	3.087	325	328	332	rVV2	352	607	0.10%	0.013%
11	3.148	335	338	340	rBV	153	149	0.02%	0.003%
12	3.178	342	343	344	rBV	130	59	0.01%	0.001%
13	3.239	351	353	354	rBV2	96	96	0.02%	0.002%
14	3.270	357	358	361	rVV	126	131	0.02%	0.003%
15	3.312	364	365	366	rVB	198	72	0.01%	0.001%
16	3.367	372	374	377	rVB2	100	73	0.01%	0.002%
17	3.428	382	384	392	rVB3	507	1036	0.16%	0.021%
18	3.501	392	396	397	rBV2	161	241	0.04%	0.005%
19	3.556	404	405	408	rBV2	117	114	0.02%	0.002%
20	3.794	443	444	445	rVB	106	39	0.01%	0.001%
21	3.885	457	459	460	rBV	79	56	0.01%	0.001%
22	3.946	468	469	471	rBV2	113	90	0.01%	0.002%
23	3.983	474	475	477	rVV	172	109	0.02%	0.002%
24	4.026	480	482	486	rVV	129	150	0.02%	0.003%
25	4.093	490	493	496	rBV2	135	216	0.03%	0.004%
26	4.196	509	510	511	rBV	112	57	0.01%	0.001%
27	4.282	521	524	525	rBV2	270	224	0.04%	0.005%
28	4.465	546	554	569	rBV	45107	135420	21.43%	2.806%
29	4.696	588	592	595	rBV5	791	1618	0.26%	0.034%
30	4.891	623	624	625	rBV	134	54	0.01%	0.001%
31	4.934	629	631	633	rBV	116	101	0.02%	0.002%
32	5.056	639	651	666	rBV	81107	250154	39.58%	5.184%
33	5.202	673	675	677	rBV2	193	211	0.03%	0.004%
34	5.464	714	718	720	rBV2	234	382	0.06%	0.008%
35	5.544	728	731	733	rBV3	219	319	0.05%	0.007%
36	5.672	750	752	753	rBV	126	55	0.01%	0.001%

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 Title : VOC Analysis

37	5.794	770	772	773	rBV	79	64	0.01%	0.001%
38	5.964	789	800	818	rBV2	213562	631961	100.00%	13.096%
39	6.275	850	851	853	rVB	110	76	0.01%	0.002%
40	6.294	853	854	857	rBV	232	165	0.03%	0.003%
41	6.348	861	863	864	rBV2	93	54	0.01%	0.001%
42	6.489	884	886	888	rBV	104	93	0.01%	0.002%
43	6.556	896	897	899	rBV	125	71	0.01%	0.001%
44	6.763	922	931	943	rBV	164240	405171	64.11%	8.397%
45	7.123	986	990	991	rBV4	908	1151	0.18%	0.024%
46	7.312	1012	1021	1038	rBV	125665	284620	45.04%	5.898%
47	7.580	1063	1065	1066	rBV2	153	128	0.02%	0.003%
48	7.958	1123	1127	1130	rBV3	316	582	0.09%	0.012%
49	8.177	1161	1163	1166	rBV2	103	97	0.02%	0.002%
50	8.324	1182	1187	1199	rBV	73913	125631	19.88%	2.604%
51	8.586	1228	1230	1231	rBV	137	60	0.01%	0.001%
52	8.647	1234	1240	1250	rBV	319142	509556	80.63%	10.560%
53	8.952	1285	1290	1301	rBV	52526	80928	12.81%	1.677%
54	9.122	1317	1318	1324	rBV2	220	349	0.06%	0.007%
55	9.275	1339	1343	1349	rBV2	4229	6526	1.03%	0.135%
56	9.391	1356	1362	1377	rBV	191960	296530	46.92%	6.145%
57	9.702	1411	1413	1414	rBB2	117	70	0.01%	0.001%
58	9.860	1438	1439	1441	rVB	190	117	0.02%	0.002%
59	10.055	1465	1471	1489	rBV	343645	464049	73.43%	9.617%
60	10.201	1491	1495	1502	rVV4	773	1576	0.25%	0.033%
61	10.256	1502	1504	1508	rVV2	159	194	0.03%	0.004%
62	10.311	1508	1513	1520	rVB3	1073	1949	0.31%	0.040%
63	10.543	1550	1551	1552	rVB	88	32	0.01%	0.001%
64	10.646	1565	1568	1572	rVB2	724	892	0.14%	0.018%
65	10.683	1572	1574	1575	rBV	155	105	0.02%	0.002%
66	10.970	1617	1621	1623	rBV2	304	352	0.06%	0.007%
67	11.049	1633	1634	1635	rBV	96	49	0.01%	0.001%
68	11.092	1640	1641	1642	rBV	125	58	0.01%	0.001%
69	11.189	1652	1657	1669	rBV	251592	325252	51.47%	6.740%
70	11.384	1687	1689	1691	rVB	213	137	0.02%	0.003%
71	11.530	1711	1713	1714	rBV	108	57	0.01%	0.001%
72	11.628	1727	1729	1730	rVB	165	97	0.02%	0.002%
73	11.646	1730	1732	1733	rBV2	148	141	0.02%	0.003%
74	11.756	1746	1750	1756	rVB2	528	897	0.14%	0.019%
75	11.945	1780	1781	1782	rBV	183	75	0.01%	0.002%
76	12.024	1788	1794	1803	rBV	321688	415071	65.68%	8.602%

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77	12.219	1822	1826	1837	rBV2	4367	6073	0.96%	0.126%
78	12.317	1837	1842	1854	rVV	347507	444711	70.37%	9.216%
79	12.506	1871	1873	1875	rVB2	160	96	0.02%	0.002%
80	12.530	1875	1877	1878	rBV	123	65	0.01%	0.001%
81	12.762	1914	1915	1917	rVB	217	94	0.01%	0.002%
82	12.780	1917	1918	1920	rBV	96	48	0.01%	0.001%
83	12.951	1944	1946	1949	rVB2	140	130	0.02%	0.003%
84	13.036	1958	1960	1964	rBV	113	132	0.02%	0.003%
85	13.494	2034	2035	2036	rBV	223	94	0.01%	0.002%
86	13.695	2066	2068	2071	rBV	138	135	0.02%	0.003%
87	13.780	2079	2082	2083	rBV	356	378	0.06%	0.008%
88	14.024	2120	2122	2124	rBV2	185	182	0.03%	0.004%
89	14.134	2136	2140	2143	rBV	575	760	0.12%	0.016%
90	14.335	2171	2173	2175	rBV2	163	185	0.03%	0.004%

Sum of corrected areas: 4825436

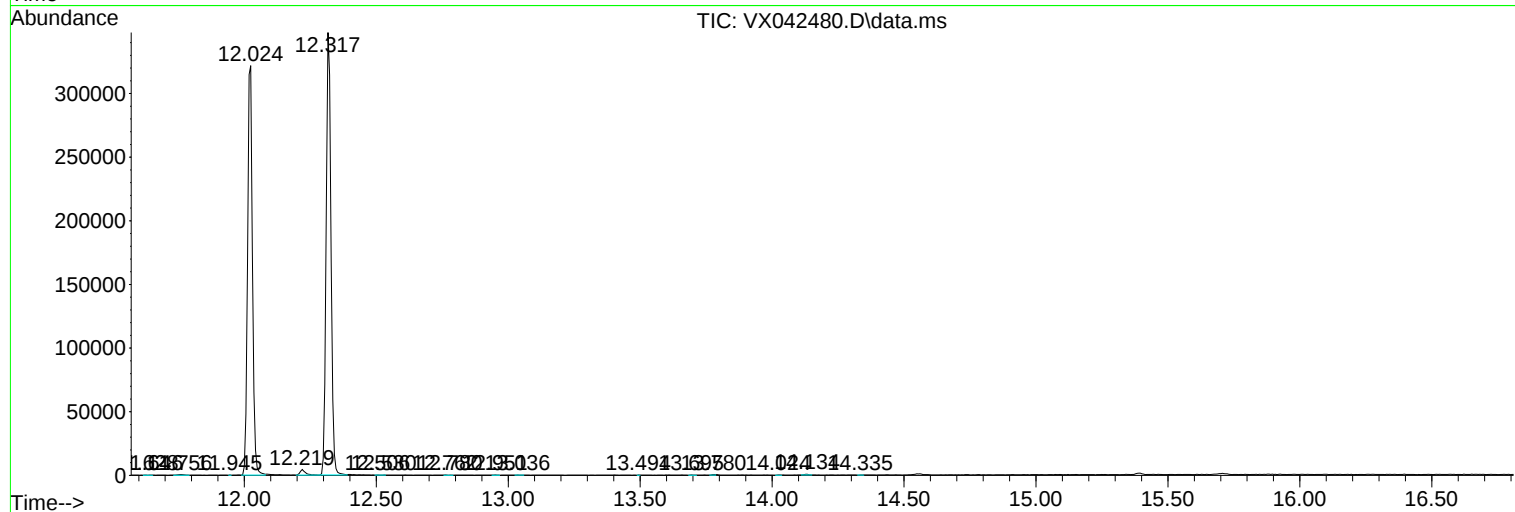
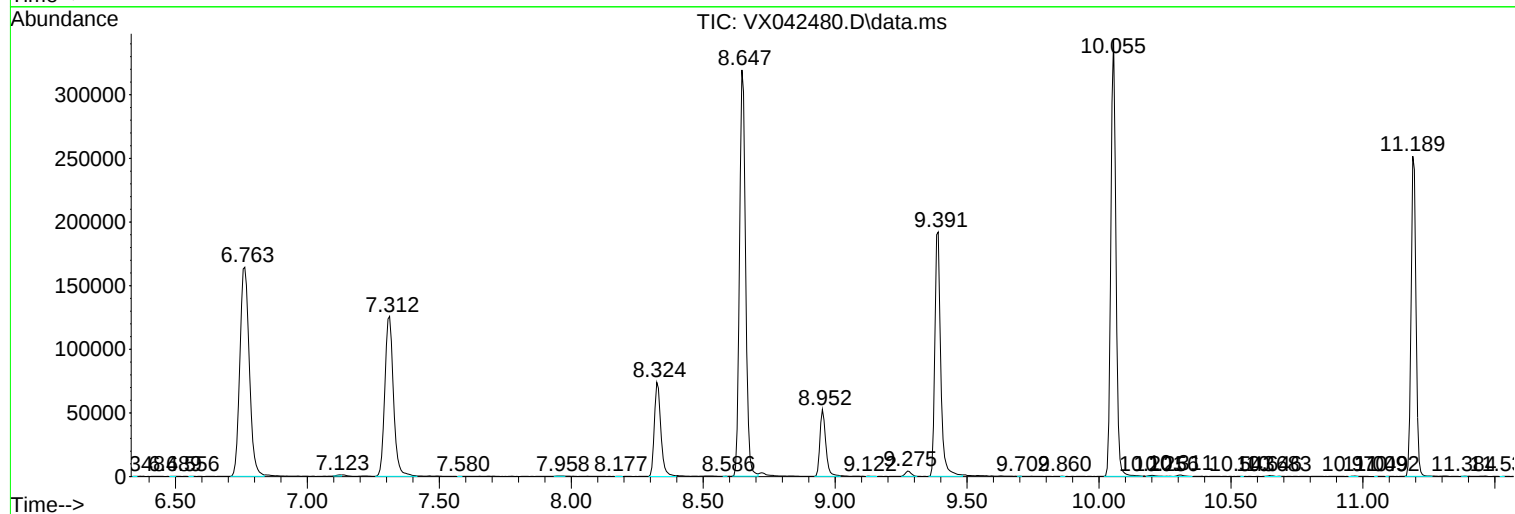
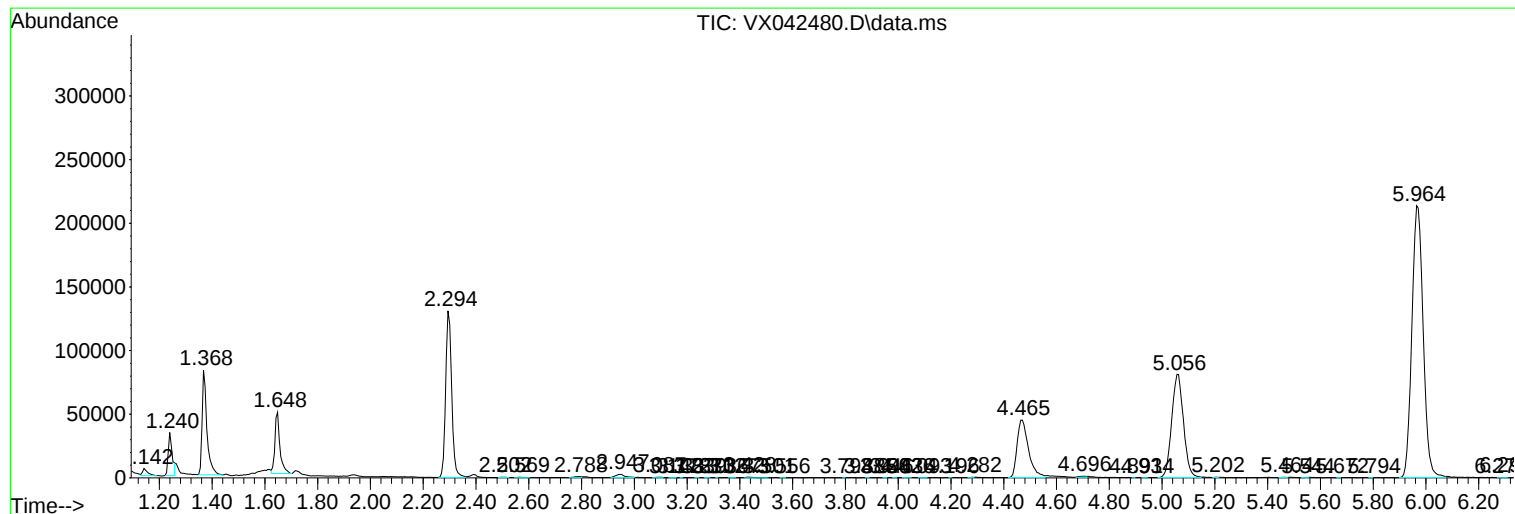
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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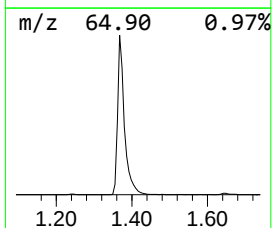
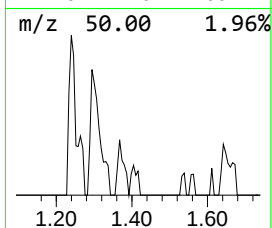
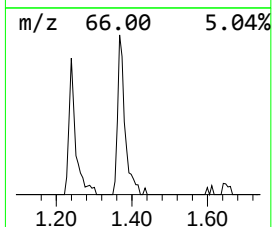
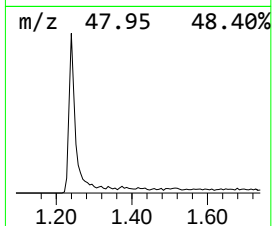
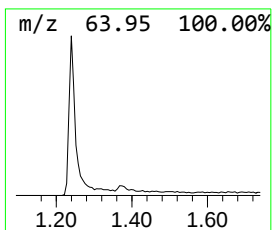
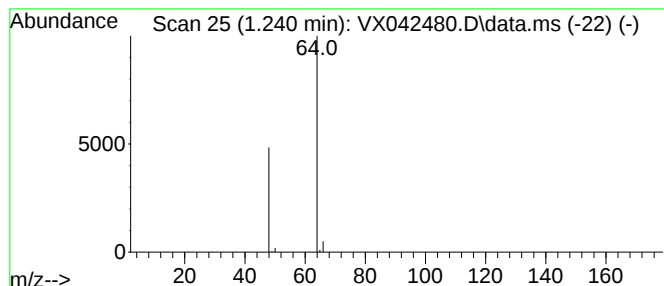
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	4.42 ug/L	35843	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	4.4	ug/L	35843	1	6.763	405171	50.0