

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042481.D
 Acq On : 23 Jul 2024 18:50
 Operator : JC/MD
 Sample : P3327-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZW7

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: VX042481.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	20	rVB	9064	11961	2.08%	0.264%
2	1.240	22	25	28	rBV	26102	28445	4.95%	0.628%
3	1.368	43	46	58	rVB	47172	61397	10.68%	1.355%
4	1.648	88	92	100	rVB	39450	51324	8.93%	1.133%
5	1.721	101	104	115	rVB2	8021	12505	2.18%	0.276%
6	1.935	136	139	144	rVB2	3732	4909	0.85%	0.108%
7	2.294	192	198	209	rBV	98195	158392	27.55%	3.496%
8	2.398	211	215	222	rVB3	1189	2210	0.38%	0.049%
9	2.502	229	232	234	rBV	260	268	0.05%	0.006%
10	2.569	237	243	250	rBV3	475	1000	0.17%	0.022%
11	2.685	257	262	263	rBV2	114	149	0.03%	0.003%
12	2.703	263	265	268	rBV	156	178	0.03%	0.004%
13	2.782	271	278	279	rBV5	1114	1614	0.28%	0.036%
14	2.941	298	304	310	rBV3	700	1697	0.30%	0.037%
15	3.093	324	329	336	rVB3	806	1622	0.28%	0.036%
16	3.215	346	349	351	rVB2	112	146	0.03%	0.003%
17	3.441	380	386	393	rVV4	1214	2481	0.43%	0.055%
18	3.977	471	474	476	rBV	110	153	0.03%	0.003%
19	4.014	479	480	482	rBV	177	125	0.02%	0.003%
20	4.300	519	527	535	rVB5	946	2379	0.41%	0.053%
21	4.465	546	554	574	rBV	44748	135813	23.62%	2.998%
22	5.056	639	651	671	rBV	73710	230119	40.03%	5.079%
23	5.397	704	707	710	rBV3	251	429	0.07%	0.009%
24	5.465	713	718	719	rBV3	670	841	0.15%	0.019%
25	5.666	750	751	754	rVB	148	108	0.02%	0.002%
26	5.739	759	763	765	rBV2	151	162	0.03%	0.004%
27	5.818	774	776	777	rBV	163	107	0.02%	0.002%
28	5.971	790	801	822	rBV2	193007	574900	100.00%	12.689%
29	6.361	861	865	869	rVB3	335	490	0.09%	0.011%
30	6.501	885	888	889	rBV2	134	156	0.03%	0.003%
31	6.544	892	895	897	rBV2	106	143	0.02%	0.003%
32	6.617	903	907	911	rVB	358	428	0.07%	0.009%
33	6.763	922	931	948	rBV	172402	410926	71.48%	9.070%
34	7.135	984	992	1003	rVB4	3016	7483	1.30%	0.165%
35	7.220	1003	1006	1007	rBV2	195	198	0.03%	0.004%
36	7.312	1012	1021	1043	rBV	115269	264637	46.03%	5.841%

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Integrator: RTE

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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

37	7.476	1046	1048	1049	rBV2	199	154	0.03%	0.003%
38	7.635	1073	1074	1080	rBV2	82	125	0.02%	0.003%
39	7.793	1097	1100	1101	rBV	141	125	0.02%	0.003%
40	7.897	1114	1117	1119	rVB	166	139	0.02%	0.003%
41	7.964	1122	1128	1131	rBV2	592	1294	0.23%	0.029%
42	8.068	1144	1145	1148	rVB	165	111	0.02%	0.002%
43	8.263	1174	1177	1178	rVV2	169	139	0.02%	0.003%
44	8.281	1178	1180	1181	rVV	122	121	0.02%	0.003%
45	8.324	1182	1187	1200	rVV	65077	111932	19.47%	2.471%
46	8.427	1202	1204	1208	rVB3	337	301	0.05%	0.007%
47	8.501	1214	1216	1217	rBV2	169	174	0.03%	0.004%
48	8.519	1217	1219	1220	rVV	285	186	0.03%	0.004%
49	8.592	1228	1231	1234	rBV2	570	754	0.13%	0.017%
50	8.647	1234	1240	1249	rVV	278346	444652	77.34%	9.814%
51	8.726	1249	1253	1263	rVB	6043	11617	2.02%	0.256%
52	8.952	1285	1290	1302	rBV	47636	72053	12.53%	1.590%
53	9.086	1311	1312	1315	rBV2	162	161	0.03%	0.004%
54	9.275	1338	1343	1349	rBV	3990	5740	1.00%	0.127%
55	9.385	1356	1361	1382	rBV	188651	290216	50.48%	6.405%
56	9.763	1420	1423	1427	rBV	210	271	0.05%	0.006%
57	10.055	1465	1471	1490	rBV	345638	470971	81.92%	10.395%
58	10.202	1491	1495	1500	rVB	2338	3047	0.53%	0.067%
59	10.305	1507	1512	1525	rBV	3385	5420	0.94%	0.120%
60	10.488	1540	1542	1544	rBV2	111	133	0.02%	0.003%
61	10.531	1546	1549	1551	rBV2	101	157	0.03%	0.003%
62	10.647	1564	1568	1575	rVB2	1211	1877	0.33%	0.041%
63	10.787	1589	1591	1593	rBV	167	157	0.03%	0.003%
64	10.860	1600	1603	1605	rBV2	117	106	0.02%	0.002%
65	10.970	1617	1621	1624	rBV3	356	399	0.07%	0.009%
66	11.189	1652	1657	1669	rBV	237310	311297	54.15%	6.871%
67	11.384	1684	1689	1691	rBV3	533	679	0.12%	0.015%
68	11.457	1696	1701	1704	rBV2	653	855	0.15%	0.019%
69	11.506	1708	1709	1713	rVB2	110	105	0.02%	0.002%
70	11.616	1724	1727	1732	rBV	296	411	0.07%	0.009%
71	11.756	1746	1750	1755	rBV3	1557	1993	0.35%	0.044%
72	11.976	1782	1786	1788	rBV2	196	194	0.03%	0.004%
73	12.024	1788	1794	1802	rBV	317819	412202	71.70%	9.098%
74	12.177	1817	1819	1820	rVB	246	142	0.02%	0.003%
75	12.219	1822	1826	1833	rVV2	5416	7142	1.24%	0.158%
76	12.274	1833	1835	1837	rVV	248	215	0.04%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Sampling : 1

Min Area: 0 % of largest Peak

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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

77	12.317	1837	1842	1863	rVV	304637	397434	69.13%	8.772%
78	12.469	1865	1867	1870	rBV3	215	307	0.05%	0.007%
79	12.610	1889	1890	1893	rVB2	188	168	0.03%	0.004%
80	12.707	1903	1906	1908	rBV2	156	200	0.03%	0.004%
81	12.762	1913	1915	1919	rBV2	309	358	0.06%	0.008%
82	12.847	1927	1929	1935	rVV3	112	176	0.03%	0.004%
83	12.921	1939	1941	1943	rVB2	185	142	0.02%	0.003%
84	12.969	1945	1949	1952	rVV2	293	355	0.06%	0.008%
85	13.024	1955	1958	1962	rVB2	166	216	0.04%	0.005%
86	13.286	1998	2001	2006	rVV3	207	292	0.05%	0.006%
87	13.524	2039	2040	2043	rVB2	119	104	0.02%	0.002%
88	13.731	2072	2074	2077	rVV2	162	165	0.03%	0.004%
89	13.780	2077	2082	2089	rVB3	517	903	0.16%	0.020%
90	13.841	2089	2092	2093	rBV2	171	151	0.03%	0.003%
91	13.884	2096	2099	2102	rBV2	147	217	0.04%	0.005%
92	14.091	2131	2133	2135	rBV2	135	124	0.02%	0.003%
93	14.109	2135	2136	2137	rVV	223	141	0.02%	0.003%
94	14.134	2137	2140	2145	rVB3	414	522	0.09%	0.012%
95	14.237	2156	2157	2160	rVB2	163	108	0.02%	0.002%
96	14.268	2160	2162	2165	rBV3	184	211	0.04%	0.005%
97	14.597	2214	2216	2218	rBV3	222	166	0.03%	0.004%
98	14.646	2223	2224	2227	rVB2	321	208	0.04%	0.005%
99	14.835	2253	2255	2256	rBV2	260	135	0.02%	0.003%
100	16.176	2473	2475	2477	rBV	388	268	0.05%	0.006%

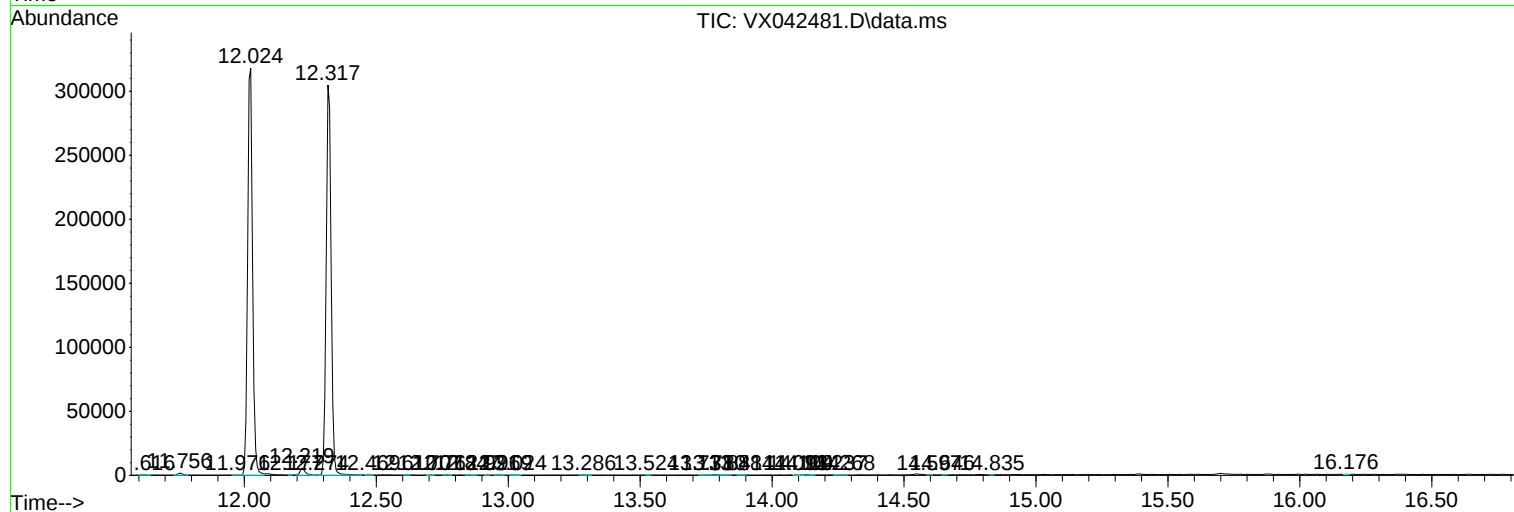
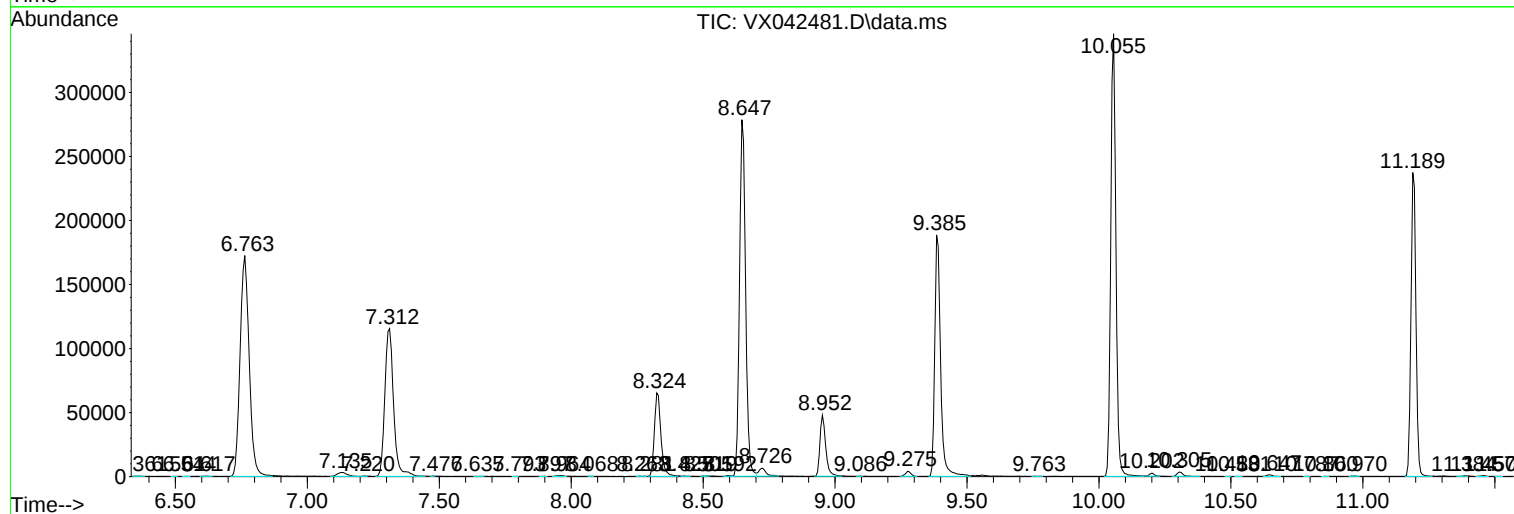
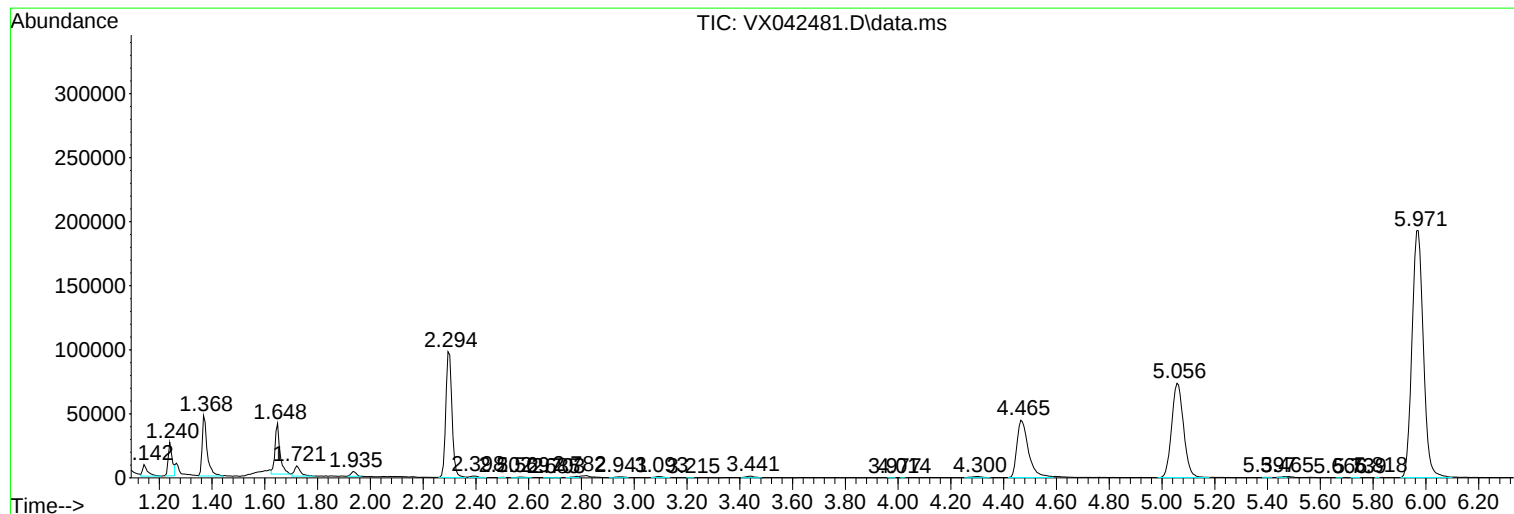
Sum of corrected areas: 4530733

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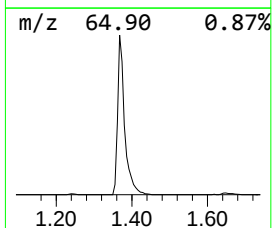
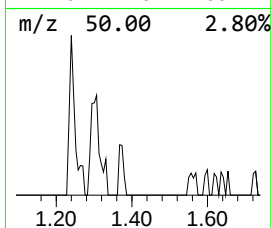
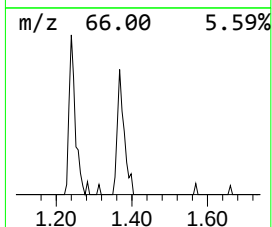
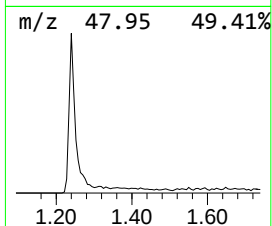
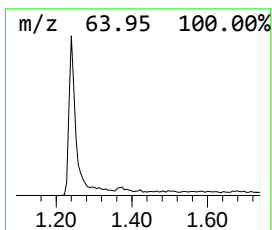
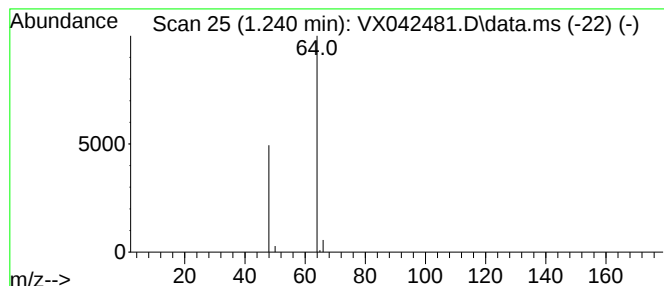
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.46 ug/L	28445	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			Sulfur dioxide	64	O2S	007446-09-5	4



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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	1.240	3.5	ug/L	28445	1	6.763	410926	50.0