

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042587.D
 Acq On : 25 Jul 2024 23:09
 Operator : JC/MD
 Sample : P3328-06ME 20X
 Misc : 8.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZT9ME

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: VX042587.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	36	rBV	18289	24984	4.37%	0.568%
2	1.368	43	46	57	rVB	47120	59736	10.45%	1.357%
3	1.563	70	78	79	rBV3	2303	4108	0.72%	0.093%
4	1.648	88	92	102	rVB	41398	56109	9.81%	1.275%
5	1.935	138	139	141	rVB	386	142	0.02%	0.003%
6	2.148	172	174	179	rVB4	422	526	0.09%	0.012%
7	2.294	192	198	210	rVB	106926	170579	29.83%	3.876%
8	2.380	210	212	213	rBV2	169	167	0.03%	0.004%
9	2.502	229	232	237	rBV3	390	717	0.13%	0.016%
10	2.575	241	244	245	rBV	177	167	0.03%	0.004%
11	2.648	254	256	259	rBV2	172	233	0.04%	0.005%
12	2.715	263	267	268	rVV3	189	218	0.04%	0.005%
13	2.788	272	279	288	rBV3	2450	5283	0.92%	0.120%
14	2.941	296	304	317	rVB2	5955	14289	2.50%	0.325%
15	3.184	341	344	347	rBV	99	149	0.03%	0.003%
16	3.282	357	360	361	rBV	131	129	0.02%	0.003%
17	3.386	376	377	381	rVB	192	206	0.04%	0.005%
18	3.422	381	383	384	rBV	164	148	0.03%	0.003%
19	3.434	384	385	389	rVV2	128	149	0.03%	0.003%
20	3.501	394	396	399	rVB	190	176	0.03%	0.004%
21	3.684	422	426	427	rBV	149	165	0.03%	0.004%
22	3.879	456	458	461	rBV	100	166	0.03%	0.004%
23	4.099	493	494	497	rBV2	140	173	0.03%	0.004%
24	4.160	502	504	506	rBV	150	151	0.03%	0.003%
25	4.270	521	522	526	rBV2	113	147	0.03%	0.003%
26	4.385	539	541	542	rBV	182	131	0.02%	0.003%
27	4.465	546	554	569	rBV	42456	126808	22.18%	2.882%
28	4.800	606	609	612	rVB3	151	228	0.04%	0.005%
29	4.824	612	613	616	rBV3	134	158	0.03%	0.004%
30	5.062	637	652	669	rBV	73102	228426	39.95%	5.191%
31	5.221	677	678	680	rVB	183	127	0.02%	0.003%
32	5.245	680	682	684	rBB	149	127	0.02%	0.003%
33	5.294	688	690	693	rVV	252	176	0.03%	0.004%
34	5.391	702	706	709	rBV3	217	321	0.06%	0.007%
35	5.550	730	732	735	rBV	194	225	0.04%	0.005%
36	5.653	747	749	753	rVB	158	180	0.03%	0.004%

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

37	5.708	755	758	762	rVB2	91	150	0.03%	0.003%
38	5.964	789	800	818	rBV2	194409	571844	100.00%	12.994%
39	6.300	852	855	859	rVB2	119	215	0.04%	0.005%
40	6.763	921	931	946	rBV	166816	406495	71.08%	9.237%
41	6.934	958	959	961	rBV2	165	129	0.02%	0.003%
42	7.050	976	978	979	rVB2	195	136	0.02%	0.003%
43	7.129	983	991	1000	rVV4	8133	20029	3.50%	0.455%
44	7.214	1003	1005	1008	rVV2	343	380	0.07%	0.009%
45	7.306	1012	1020	1043	rVV	118547	258557	45.21%	5.875%
46	7.623	1070	1072	1074	rBV2	166	135	0.02%	0.003%
47	7.678	1079	1081	1085	rVB2	151	227	0.04%	0.005%
48	7.720	1085	1088	1091	rBV2	132	191	0.03%	0.004%
49	7.848	1106	1109	1110	rBV2	170	161	0.03%	0.004%
50	8.110	1151	1152	1155	rVB	207	173	0.03%	0.004%
51	8.324	1181	1187	1204	rVV	65402	111424	19.49%	2.532%
52	8.555	1223	1225	1230	rBV2	155	290	0.05%	0.007%
53	8.647	1234	1240	1256	rVV	275487	439748	76.90%	9.993%
54	8.952	1285	1290	1301	rBV	47448	71987	12.59%	1.636%
55	9.110	1314	1316	1317	rBV	176	127	0.02%	0.003%
56	9.275	1340	1343	1348	rVB2	1474	1901	0.33%	0.043%
57	9.385	1356	1361	1381	rBV	184738	277041	48.45%	6.295%
58	9.702	1408	1413	1417	rBV2	1328	2143	0.37%	0.049%
59	9.775	1423	1425	1427	rBV	214	273	0.05%	0.006%
60	9.823	1430	1433	1434	rVV2	130	157	0.03%	0.004%
61	9.836	1434	1435	1439	rVB2	171	160	0.03%	0.004%
62	9.915	1446	1448	1449	rBV	187	151	0.03%	0.003%
63	10.055	1465	1471	1486	rBV	329923	461905	80.77%	10.496%
64	10.183	1490	1492	1494	rBV2	171	169	0.03%	0.004%
65	10.317	1510	1514	1516	rBV4	358	466	0.08%	0.011%
66	10.579	1555	1557	1562	rVB2	112	133	0.02%	0.003%
67	10.646	1567	1568	1574	rVV3	180	258	0.05%	0.006%
68	10.781	1587	1590	1593	rBV2	143	267	0.05%	0.006%
69	10.964	1619	1620	1624	rVB	220	212	0.04%	0.005%
70	11.104	1641	1643	1647	rBV2	136	161	0.03%	0.004%
71	11.189	1652	1657	1669	rBV	224670	297924	52.10%	6.770%
72	11.317	1674	1678	1681	rVB3	218	302	0.05%	0.007%
73	11.537	1712	1714	1717	rVB2	173	161	0.03%	0.004%
74	11.567	1717	1719	1720	rBV2	163	142	0.02%	0.003%
75	11.610	1723	1726	1727	rVV2	137	136	0.02%	0.003%
76	11.628	1727	1729	1732	rVV2	229	242	0.04%	0.005%

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

77	11.969	1781	1785	1788	rBV2	258	419	0.07%	0.010%
78	12.024	1788	1794	1807	rVV	297726	392463	68.63%	8.918%
79	12.317	1837	1842	1853	rBV	295040	380314	66.51%	8.642%
80	12.482	1866	1869	1873	rVB3	167	209	0.04%	0.005%
81	12.536	1876	1878	1881	rBV	267	308	0.05%	0.007%
82	12.762	1911	1915	1920	rBV3	355	582	0.10%	0.013%
83	12.920	1939	1941	1945	rBV2	139	160	0.03%	0.004%
84	13.122	1971	1974	1976	rVB3	175	217	0.04%	0.005%
85	13.433	2023	2025	2029	rBV2	109	167	0.03%	0.004%
86	13.591	2049	2051	2052	rBV	294	183	0.03%	0.004%
87	13.701	2067	2069	2070	rBV	130	128	0.02%	0.003%
88	13.786	2079	2083	2085	rBV2	391	447	0.08%	0.010%
89	13.969	2111	2113	2114	rVV	294	132	0.02%	0.003%
90	14.128	2136	2139	2143	rBV3	198	291	0.05%	0.007%
91	14.451	2190	2192	2195	rBV3	170	247	0.04%	0.006%
92	14.499	2198	2200	2203	rVB2	191	185	0.03%	0.004%
93	14.591	2213	2215	2217	rBV2	238	235	0.04%	0.005%
94	15.085	2295	2296	2298	rVB	227	128	0.02%	0.003%
95	15.176	2310	2311	2312	rBV	194	133	0.02%	0.003%
96	15.481	2358	2361	2364	rBV4	266	382	0.07%	0.009%
97	15.743	2403	2404	2407	rVB2	305	223	0.04%	0.005%
98	15.902	2429	2430	2432	rVB	276	135	0.02%	0.003%
99	16.560	2536	2538	2541	rBV2	232	254	0.04%	0.006%
100	16.658	2553	2554	2555	rBV	290	126	0.02%	0.003%

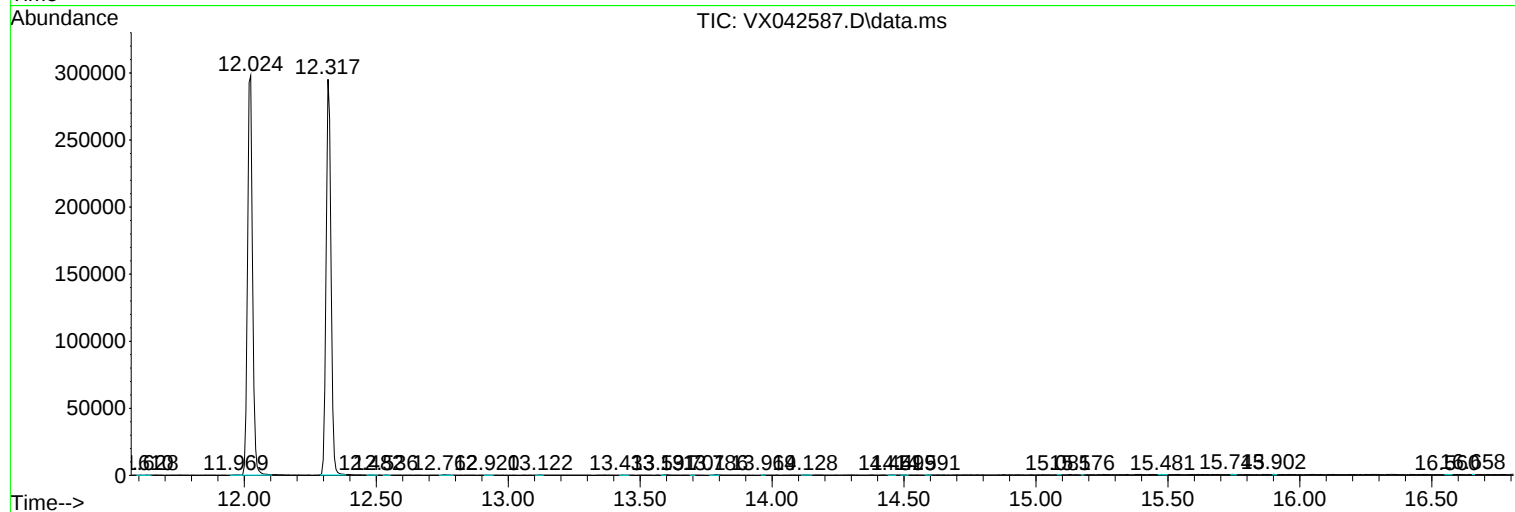
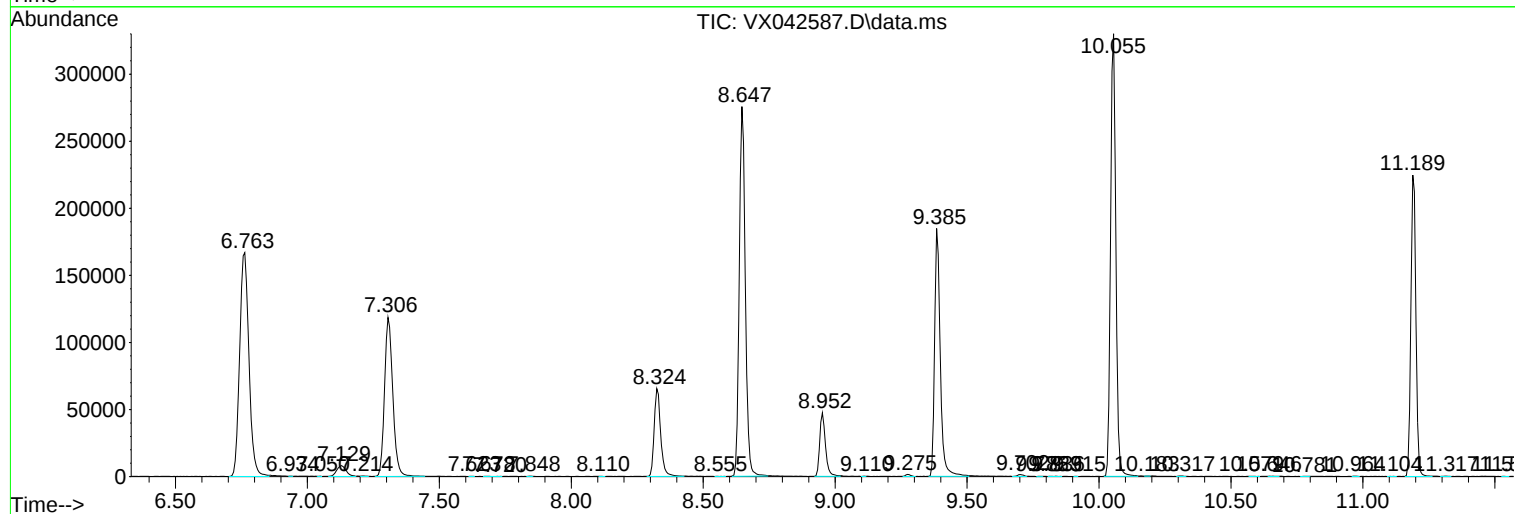
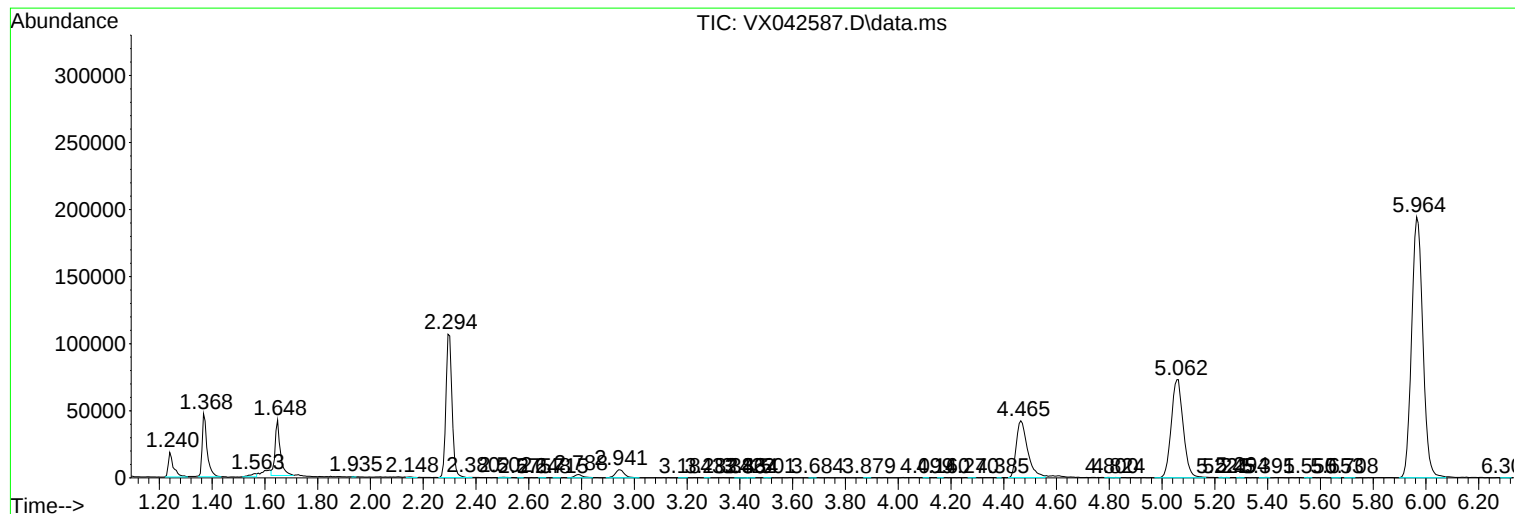
Sum of corrected areas: 4400694

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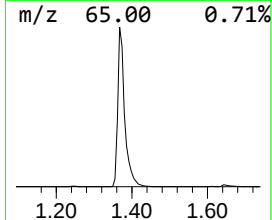
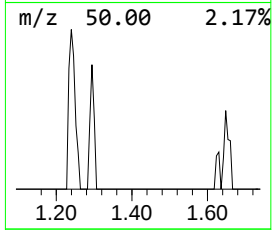
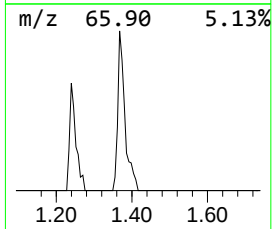
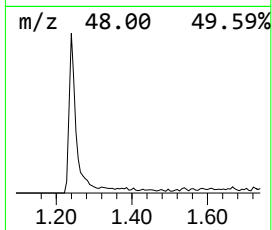
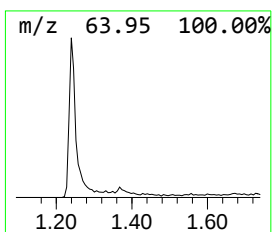
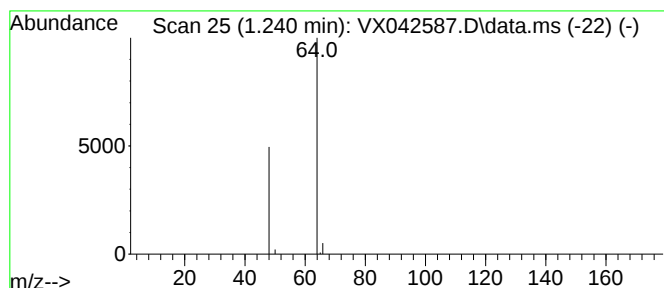
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.07 ug/L	24984	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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.1	ug/L	24984	1	6.763	406495	50.0