

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042425.D
 Acq On : 20 Jul 2024 00:16
 Operator : JC/MD
 Sample : P3298-14 100X
 Misc : 5.13g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BHB44

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: VX042425.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	37	rBV	29270	40586	6.10%	0.775%
2	1.368	43	46	57	rVB	57622	76632	11.52%	1.463%
3	1.648	88	92	103	rVB	47330	67231	10.10%	1.284%
4	2.294	192	198	211	rBV	114944	186304	28.00%	3.557%
5	2.380	211	212	214	rBV2	290	294	0.04%	0.006%
6	2.502	230	232	234	rBV	317	222	0.03%	0.004%
7	2.636	252	254	256	rVB2	154	112	0.02%	0.002%
8	2.672	258	260	262	rBV2	162	132	0.02%	0.003%
9	2.715	264	267	271	rBV2	271	505	0.08%	0.010%
10	2.788	274	279	284	rVB3	704	1293	0.19%	0.025%
11	2.947	298	305	312	rVB	2098	4826	0.73%	0.092%
12	3.160	338	340	343	rBV2	101	121	0.02%	0.002%
13	3.282	356	360	362	rBV2	167	244	0.04%	0.005%
14	3.312	362	365	370	rVB2	167	191	0.03%	0.004%
15	3.404	377	380	386	rBV2	172	378	0.06%	0.007%
16	3.495	391	395	397	rBV2	130	167	0.03%	0.003%
17	3.629	413	417	418	rVB2	149	147	0.02%	0.003%
18	3.751	435	437	443	rVB2	183	285	0.04%	0.005%
19	3.934	464	467	468	rBV	125	119	0.02%	0.002%
20	4.099	493	494	497	rVB	185	128	0.02%	0.002%
21	4.123	497	498	501	rBV2	211	196	0.03%	0.004%
22	4.221	512	514	516	rBV2	115	140	0.02%	0.003%
23	4.270	518	522	523	rBV2	130	163	0.02%	0.003%
24	4.379	539	540	544	rVB2	178	169	0.03%	0.003%
25	4.465	546	554	571	rBV	46825	139843	21.02%	2.670%
26	4.855	616	618	619	rBV	186	160	0.02%	0.003%
27	4.897	623	625	628	rVB2	179	187	0.03%	0.004%
28	4.971	636	637	640	rBV	177	163	0.02%	0.003%
29	5.056	640	651	671	rBV2	83190	257953	38.77%	4.925%
30	5.202	674	675	677	rVB	423	229	0.03%	0.004%
31	5.227	677	679	681	rBV2	174	172	0.03%	0.003%
32	5.288	687	689	694	rBV	193	233	0.04%	0.004%
33	5.391	702	706	707	rBV2	293	390	0.06%	0.007%
34	5.617	739	743	744	rBV	170	133	0.02%	0.003%
35	5.739	761	763	766	rBV2	112	120	0.02%	0.002%
36	5.964	789	800	818	rBV2	227078	665342	100.00%	12.702%

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

37	6.342	859	862	863	rBV	162	180	0.03%	0.003%
38	6.604	903	905	908	rBV2	145	158	0.02%	0.003%
39	6.763	921	931	946	rBV	207077	505043	75.91%	9.642%
40	6.915	955	956	958	rBV	336	146	0.02%	0.003%
41	6.952	961	962	963	rBV	256	143	0.02%	0.003%
42	7.117	983	989	996	rVB5	1119	2779	0.42%	0.053%
43	7.202	1000	1003	1005	rBV	309	405	0.06%	0.008%
44	7.306	1012	1020	1036	rBV	132055	294095	44.20%	5.615%
45	7.495	1048	1051	1053	rBV2	338	323	0.05%	0.006%
46	7.543	1058	1059	1062	rBV	262	240	0.04%	0.005%
47	7.665	1077	1079	1081	rBV2	140	163	0.02%	0.003%
48	7.702	1084	1085	1087	rBV2	175	154	0.02%	0.003%
49	7.769	1094	1096	1097	rBV	131	107	0.02%	0.002%
50	7.958	1123	1127	1132	rBV3	399	820	0.12%	0.016%
51	8.214	1167	1169	1170	rBV	133	114	0.02%	0.002%
52	8.324	1181	1187	1200	rBV	69699	122068	18.35%	2.330%
53	8.482	1209	1213	1215	rBV2	302	396	0.06%	0.008%
54	8.519	1217	1219	1223	rVB2	454	632	0.09%	0.012%
55	8.647	1234	1240	1256	rBV	343930	543159	81.64%	10.369%
56	8.952	1285	1290	1303	rBV	50904	79621	11.97%	1.520%
57	9.092	1311	1313	1316	rVB	216	248	0.04%	0.005%
58	9.134	1316	1320	1322	rBV3	267	319	0.05%	0.006%
59	9.153	1322	1323	1326	rVB	150	105	0.02%	0.002%
60	9.336	1351	1353	1356	rBV	204	169	0.03%	0.003%
61	9.384	1356	1361	1386	rBV	203051	315135	47.36%	6.016%
62	9.848	1433	1437	1438	rBV2	183	199	0.03%	0.004%
63	10.055	1465	1471	1484	rBV	428608	591916	88.96%	11.300%
64	10.311	1510	1513	1515	rBV2	488	394	0.06%	0.008%
65	10.329	1515	1516	1517	rVV	303	127	0.02%	0.002%
66	10.360	1520	1521	1523	rBV	158	122	0.02%	0.002%
67	10.506	1544	1545	1548	rBV	172	140	0.02%	0.003%
68	10.646	1565	1568	1571	rBV3	221	222	0.03%	0.004%
69	10.695	1575	1576	1579	rVB2	149	133	0.02%	0.003%
70	10.970	1618	1621	1623	rBV	154	160	0.02%	0.003%
71	11.000	1625	1626	1629	rVB2	170	121	0.02%	0.002%
72	11.189	1652	1657	1665	rBV	256199	341283	51.29%	6.515%
73	11.451	1698	1700	1703	rVB2	268	255	0.04%	0.005%
74	11.549	1714	1716	1718	rBV	226	168	0.03%	0.003%
75	11.628	1726	1729	1732	rVB2	174	214	0.03%	0.004%
76	11.695	1737	1740	1742	rBV2	85	103	0.02%	0.002%

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 Title : VOC Analysis

77	11.829	1759	1762	1764	rBV2	227	219	0.03%	0.004%
78	11.908	1771	1775	1777	rBV2	113	136	0.02%	0.003%
79	12.024	1788	1794	1808	rBV	386215	508110	76.37%	9.700%
80	12.317	1837	1842	1855	rBV	370374	477439	71.76%	9.115%
81	12.591	1884	1887	1888	rVB2	131	119	0.02%	0.002%
82	12.622	1888	1892	1894	rVV2	111	151	0.02%	0.003%
83	12.859	1926	1931	1934	rBV2	137	234	0.04%	0.004%
84	13.030	1956	1959	1963	rBV3	240	419	0.06%	0.008%
85	13.207	1987	1988	1991	rVB2	155	104	0.02%	0.002%
86	13.384	2016	2017	2021	rBV2	143	164	0.02%	0.003%
87	13.463	2027	2030	2031	rBV	187	162	0.02%	0.003%
88	13.579	2047	2049	2051	rVB2	162	147	0.02%	0.003%
89	13.603	2051	2053	2054	rBV	171	143	0.02%	0.003%
90	13.640	2057	2059	2060	rBV2	175	114	0.02%	0.002%
91	13.713	2068	2071	2073	rBV	177	235	0.04%	0.004%
92	13.780	2079	2082	2086	rBV3	245	286	0.04%	0.005%
93	13.896	2099	2101	2102	rBV2	149	111	0.02%	0.002%
94	13.987	2115	2116	2117	rBV2	187	132	0.02%	0.003%
95	14.048	2124	2126	2128	rBV	191	191	0.03%	0.004%
96	14.128	2136	2139	2143	rBV2	654	904	0.14%	0.017%
97	14.323	2169	2171	2172	rBV	152	142	0.02%	0.003%
98	14.505	2200	2201	2203	rBV	266	129	0.02%	0.002%
99	15.463	2357	2358	2361	rVB2	553	255	0.04%	0.005%
100	16.389	2509	2510	2511	rBV	418	220	0.03%	0.004%

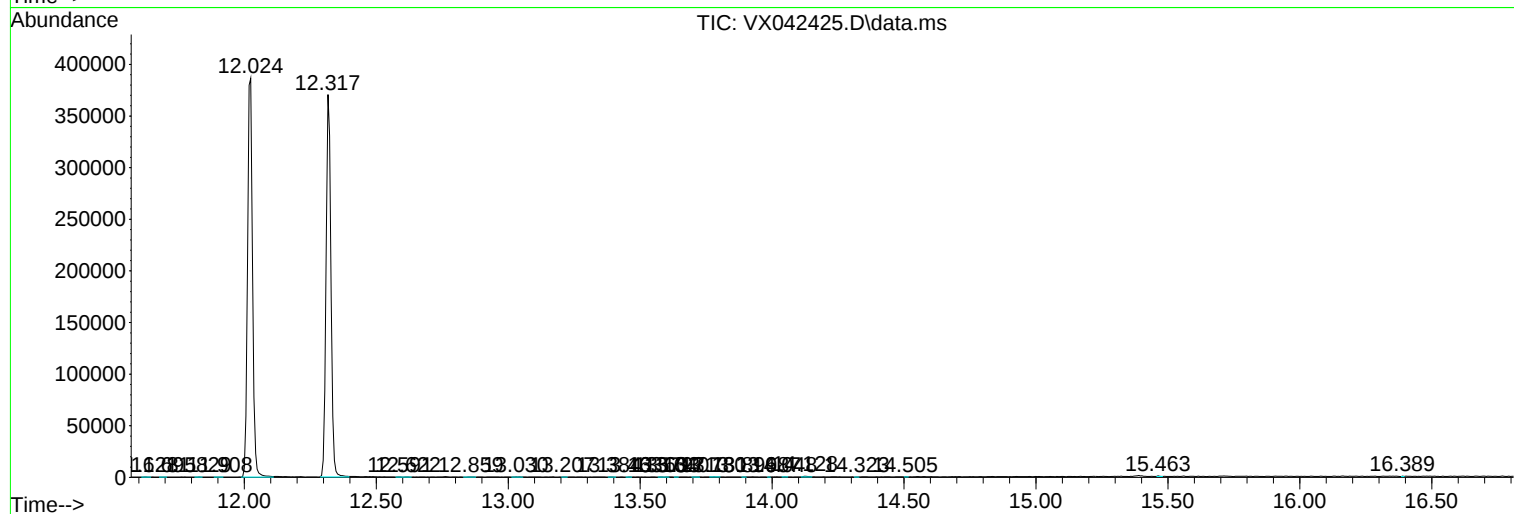
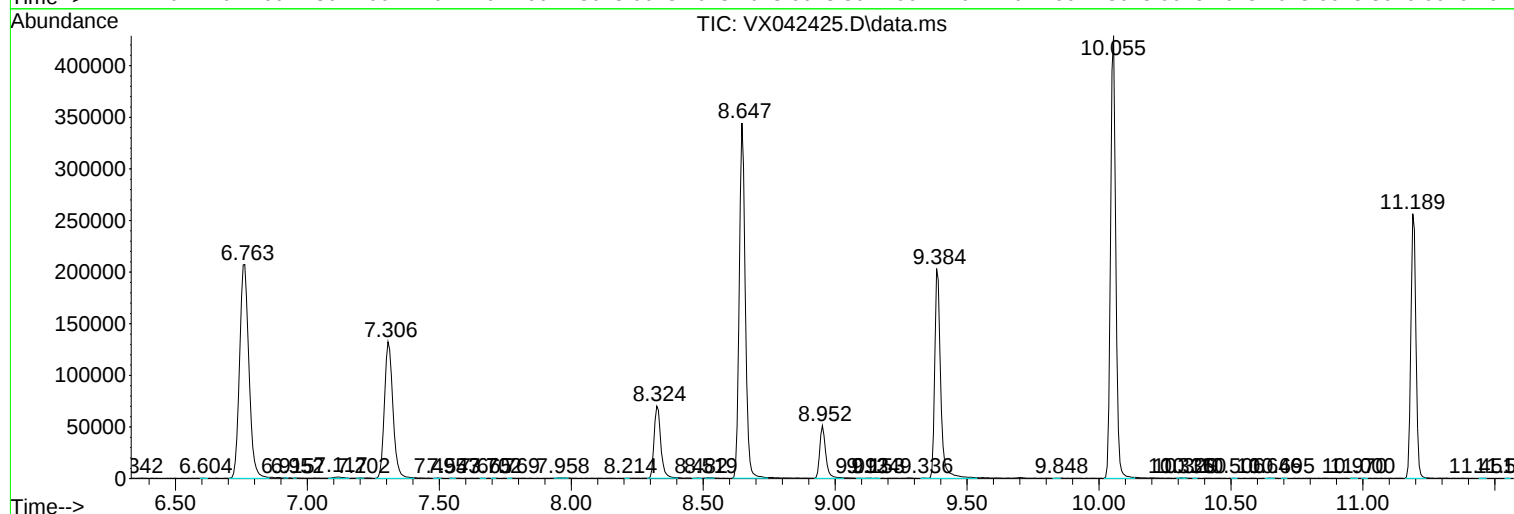
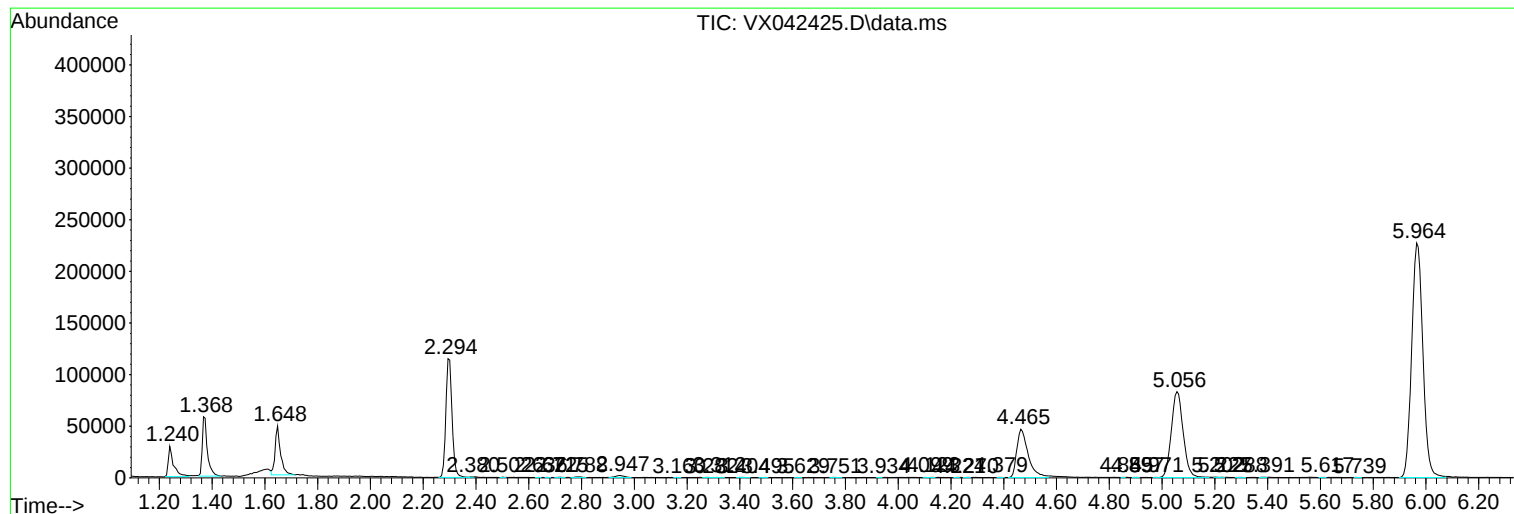
Sum of corrected areas: 5238055

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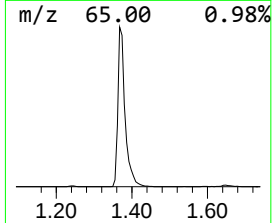
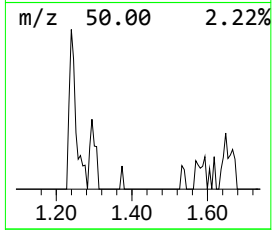
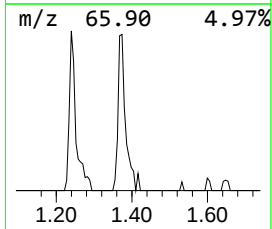
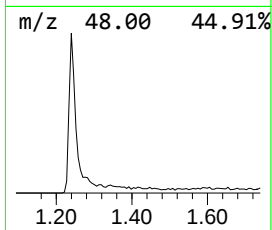
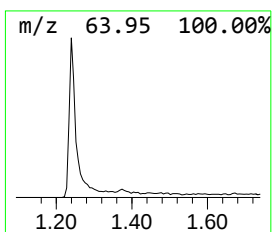
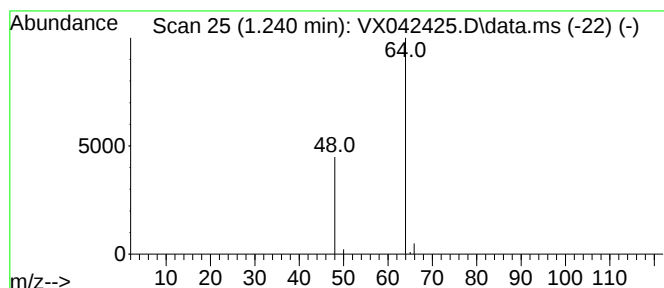
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	4.02 ug/L	40586	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	5



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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	4.0	ug/L	40586	1	6.763	505043	50.0