

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042405.D
 Acq On : 19 Jul 2024 16:29
 Operator : JC/MD
 Sample : VX0720MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK687

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: VX042405.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	39	rBV	71249	104326	11.83%	1.494%
2	1.368	43	46	59	rVV	88753	100187	11.36%	1.435%
3	1.660	90	94	110	rVB	60999	93358	10.58%	1.337%
4	2.306	193	200	210	rBV	180366	283892	32.18%	4.067%
5	2.508	229	233	240	rBV	1147	2083	0.24%	0.030%
6	2.794	274	280	287	rBV3	1629	3338	0.38%	0.048%
7	3.062	322	324	325	rBV	192	144	0.02%	0.002%
8	3.087	325	328	329	rBV2	530	591	0.07%	0.008%
9	3.203	346	347	354	rVB2	155	252	0.03%	0.004%
10	3.288	359	361	363	rBV2	197	204	0.02%	0.003%
11	3.465	387	390	393	rBV2	128	164	0.02%	0.002%
12	3.575	405	408	411	rVB2	186	216	0.02%	0.003%
13	3.611	411	414	419	rBV	277	310	0.04%	0.004%
14	3.739	433	435	438	rVB	143	165	0.02%	0.002%
15	3.831	449	450	455	rVB2	173	218	0.02%	0.003%
16	3.977	472	474	476	rBV	186	142	0.02%	0.002%
17	4.099	491	494	496	rBV2	106	131	0.01%	0.002%
18	4.459	542	553	574	rBV	65977	195303	22.14%	2.798%
19	4.800	606	609	611	rBV2	178	238	0.03%	0.003%
20	4.873	619	621	625	rVB2	159	130	0.01%	0.002%
21	4.904	625	626	629	rVB	220	146	0.02%	0.002%
22	4.934	629	631	632	rVB	212	130	0.01%	0.002%
23	4.958	632	635	639	rBV2	270	444	0.05%	0.006%
24	5.056	639	651	666	rBV	109871	339817	38.52%	4.868%
25	5.361	699	701	702	rBV	207	177	0.02%	0.003%
26	5.544	729	731	732	rVV	265	155	0.02%	0.002%
27	5.672	750	752	754	rBV3	171	163	0.02%	0.002%
28	5.964	788	800	828	rBV2	298168	882187	100.00%	12.637%
29	6.281	850	852	854	rVV2	219	191	0.02%	0.003%
30	6.312	855	857	860	rVB2	246	171	0.02%	0.002%
31	6.434	875	877	879	rVB	192	151	0.02%	0.002%
32	6.452	879	880	882	rBV	170	125	0.01%	0.002%
33	6.483	882	885	887	rBV2	165	159	0.02%	0.002%
34	6.531	892	893	894	rBV	243	130	0.01%	0.002%
35	6.629	904	909	910	rVB2	83	117	0.01%	0.002%
36	6.678	913	917	921	rBV2	94	149	0.02%	0.002%

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

37	6.757	921	930	950	rBV	259598	624111	70.75%	8.940%
38	7.117	984	989	996	rVB5	1983	4496	0.51%	0.064%
39	7.226	1003	1007	1010	rVB	211	319	0.04%	0.005%
40	7.306	1010	1020	1036	rBV	174959	388037	43.99%	5.559%
41	7.556	1059	1061	1063	rVB	149	128	0.01%	0.002%
42	7.586	1063	1066	1069	rBV	222	286	0.03%	0.004%
43	7.702	1079	1085	1086	rBV2	114	159	0.02%	0.002%
44	7.836	1101	1107	1109	rBV2	242	503	0.06%	0.007%
45	7.952	1122	1126	1130	rBV3	768	1452	0.16%	0.021%
46	8.013	1135	1136	1139	rVB2	213	159	0.02%	0.002%
47	8.043	1139	1141	1146	rVB	154	155	0.02%	0.002%
48	8.159	1157	1160	1162	rBV2	187	224	0.03%	0.003%
49	8.251	1174	1175	1178	rBV2	200	199	0.02%	0.003%
50	8.324	1181	1187	1203	rBV	103944	179038	20.29%	2.565%
51	8.507	1213	1217	1224	rBV4	578	1283	0.15%	0.018%
52	8.647	1234	1240	1251	rBV	464443	725971	82.29%	10.400%
53	8.952	1285	1290	1305	rBV	74128	113103	12.82%	1.620%
54	9.281	1339	1344	1348	rVB3	902	1396	0.16%	0.020%
55	9.384	1356	1361	1383	rBV	283866	422705	47.92%	6.055%
56	9.610	1396	1398	1402	rVB3	399	529	0.06%	0.008%
57	9.738	1417	1419	1420	rBV2	215	119	0.01%	0.002%
58	9.903	1443	1446	1449	rBV2	214	289	0.03%	0.004%
59	10.055	1465	1471	1487	rBV	505050	725763	82.27%	10.397%
60	10.195	1492	1494	1500	rVB3	1117	1575	0.18%	0.023%
61	10.311	1509	1513	1518	rVB2	1017	1602	0.18%	0.023%
62	10.457	1536	1537	1541	rBV2	102	115	0.01%	0.002%
63	10.537	1549	1550	1554	rBV	96	121	0.01%	0.002%
64	10.646	1565	1568	1570	rVV	864	1095	0.12%	0.016%
65	10.695	1574	1576	1577	rVV	197	139	0.02%	0.002%
66	10.714	1577	1579	1581	rVV2	171	150	0.02%	0.002%
67	10.750	1584	1585	1590	rVB2	169	212	0.02%	0.003%
68	10.970	1617	1621	1628	rVB2	771	1230	0.14%	0.018%
69	11.091	1638	1641	1645	rBV3	479	764	0.09%	0.011%
70	11.189	1652	1657	1669	rBV	351601	445513	50.50%	6.382%
71	11.457	1697	1701	1708	rVB3	792	1097	0.12%	0.016%
72	11.604	1724	1725	1728	rVB	180	139	0.02%	0.002%
73	11.658	1732	1734	1737	rVV	203	173	0.02%	0.002%
74	11.713	1740	1743	1745	rVV2	257	289	0.03%	0.004%
75	11.756	1747	1750	1755	rVV2	858	1109	0.13%	0.016%
76	11.915	1774	1776	1778	rBV2	127	122	0.01%	0.002%

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Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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 Title : VOC Analysis

77	11.969	1782	1785	1788	rBV	1886	2219	0.25%	0.032%
78	12.018	1788	1793	1807	rVV	512396	671495	76.12%	9.619%
79	12.183	1819	1820	1823	rVB3	295	175	0.02%	0.003%
80	12.317	1837	1842	1858	rBV	492977	630712	71.49%	9.035%
81	12.506	1871	1873	1874	rBV2	178	154	0.02%	0.002%
82	12.689	1901	1903	1905	rBV2	114	120	0.01%	0.002%
83	12.768	1911	1916	1918	rBV3	388	534	0.06%	0.008%
84	12.908	1936	1939	1943	rBV2	146	191	0.02%	0.003%
85	12.945	1943	1945	1949	rBV2	124	150	0.02%	0.002%
86	13.048	1960	1962	1967	rBV2	103	177	0.02%	0.003%
87	13.116	1968	1973	1979	rVB3	1541	2271	0.26%	0.033%
88	13.195	1984	1986	1988	rVB2	148	117	0.01%	0.002%
89	13.451	2026	2028	2029	rBV	199	158	0.02%	0.002%
90	13.524	2036	2040	2047	rBV2	230	476	0.05%	0.007%
91	13.591	2047	2051	2057	rVV3	2589	3546	0.40%	0.051%
92	13.743	2073	2076	2077	rBV3	221	273	0.03%	0.004%
93	13.780	2077	2082	2089	rVV	4044	6081	0.69%	0.087%
94	13.963	2108	2112	2117	rBV2	2514	3735	0.42%	0.054%
95	14.128	2136	2139	2146	rVB2	1125	1651	0.19%	0.024%
96	14.182	2146	2148	2150	rVB2	175	124	0.01%	0.002%
97	14.225	2153	2155	2158	rBV3	151	168	0.02%	0.002%
98	14.810	2249	2251	2252	rBV2	228	122	0.01%	0.002%
99	14.926	2268	2270	2271	rBV	243	175	0.02%	0.003%
100	16.176	2473	2475	2476	rBV	447	311	0.04%	0.004%

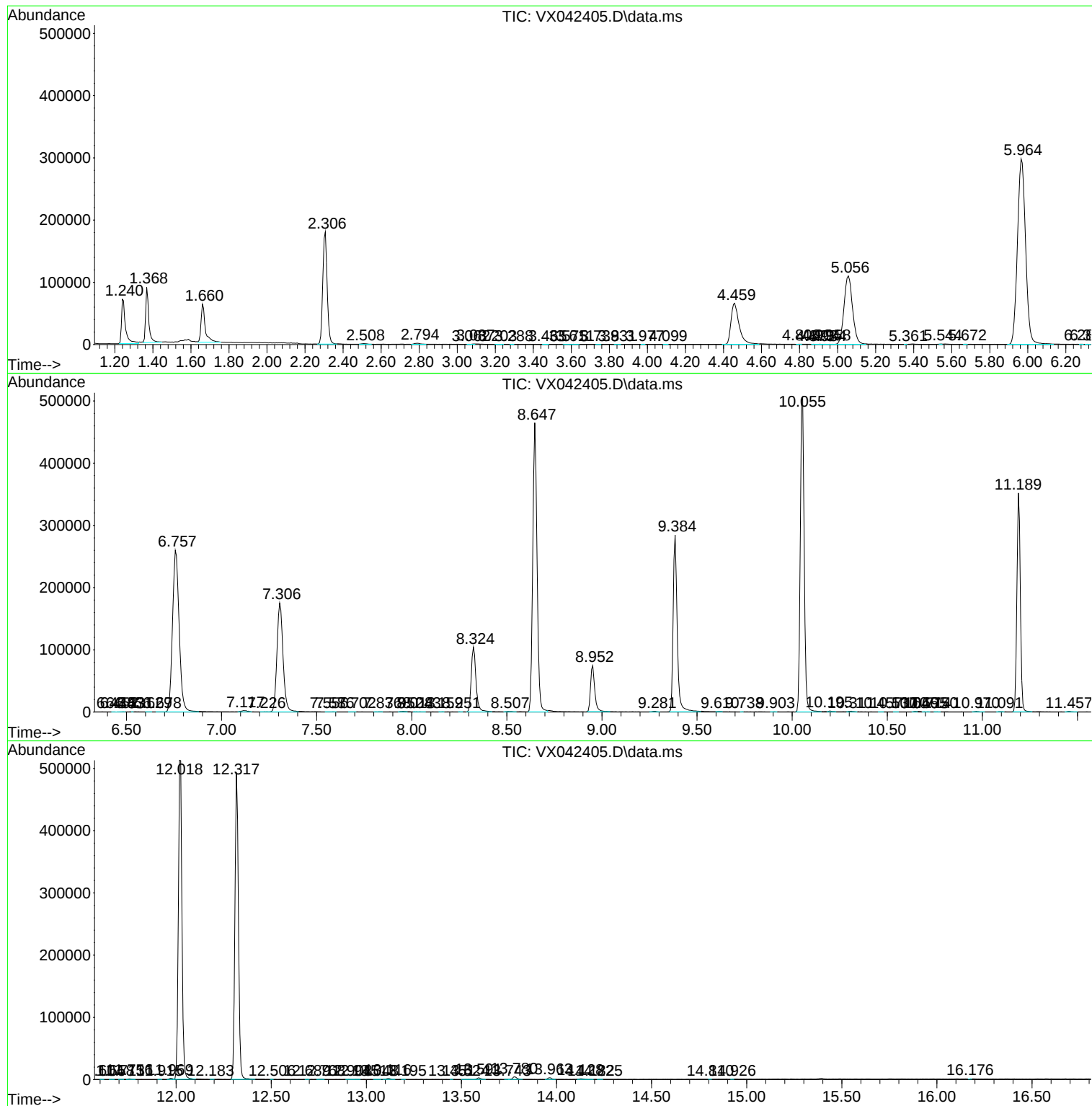
Sum of corrected areas: 6980808

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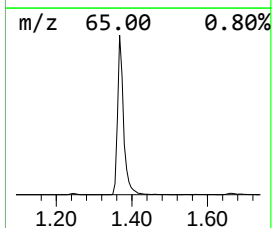
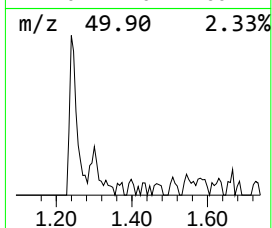
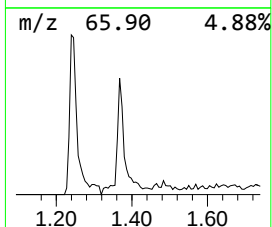
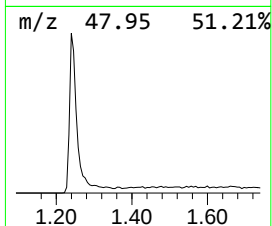
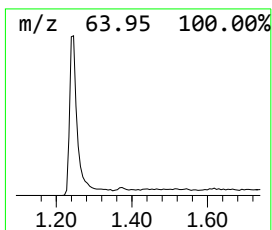
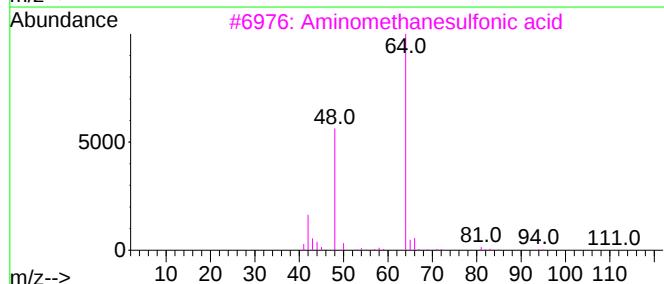
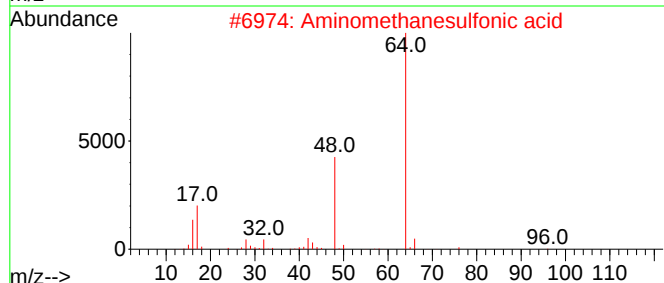
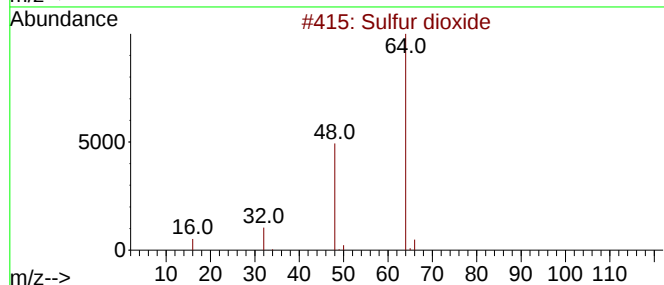
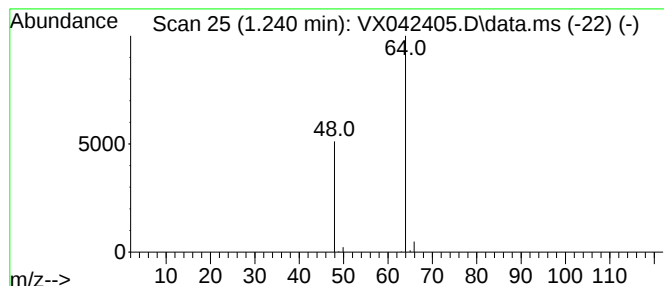
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	8.36 ug/L	104326	1,4-Difluorobenzene	6.757

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	8.4	ug/L	104326	1	6.757	624111	50.0