

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042471.D
 Acq On : 23 Jul 2024 14:57
 Operator : JC/MD
 Sample : P3263-15ME
 Misc : 5.24g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4CK3ME

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: VX042471.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	21	25	27	rBV	31293	37476	6.41%	0.768%
2	1.368	43	46	64	rVB	16294	54470	9.31%	1.116%
3	2.276	189	195	212	rBV	61358	118457	20.25%	2.427%
4	2.721	260	268	283	rBV	17558	43831	7.49%	0.898%
5	2.941	300	304	314	rVB3	2562	6150	1.05%	0.126%
6	3.069	323	325	326	rBV	152	136	0.02%	0.003%
7	3.136	332	336	339	rBV2	206	293	0.05%	0.006%
8	3.337	367	369	371	rVV2	151	111	0.02%	0.002%
9	3.465	388	390	391	rBV	120	93	0.02%	0.002%
10	3.507	395	397	399	rBV	142	147	0.03%	0.003%
11	3.605	408	413	418	rBV3	346	743	0.13%	0.015%
12	3.642	418	419	421	rVV2	109	81	0.01%	0.002%
13	3.684	424	426	429	rVV2	153	101	0.02%	0.002%
14	3.843	444	452	458	rBV2	1097	2465	0.42%	0.051%
15	3.989	474	476	478	rBV2	143	125	0.02%	0.003%
16	4.007	478	479	481	rBV	108	101	0.02%	0.002%
17	4.196	508	510	515	rBV2	113	200	0.03%	0.004%
18	4.312	528	529	531	rVB	131	78	0.01%	0.002%
19	4.330	531	532	534	rBV	150	94	0.02%	0.002%
20	4.391	540	542	544	rVB	147	114	0.02%	0.002%
21	4.428	544	548	549	rBV	117	161	0.03%	0.003%
22	4.495	551	559	576	rBV2	32864	111090	18.99%	2.276%
23	5.056	639	651	666	rBV2	71196	221973	37.94%	4.548%
24	5.373	701	703	704	rBV2	241	254	0.04%	0.005%
25	5.446	713	715	717	rBV	137	98	0.02%	0.002%
26	5.556	727	733	741	rVB3	816	2027	0.35%	0.042%
27	5.721	758	760	761	rBV	103	82	0.01%	0.002%
28	5.964	788	800	817	rBV2	203603	585006	100.00%	11.987%
29	6.269	848	850	852	rBV	159	140	0.02%	0.003%
30	6.537	892	894	895	rVB	224	126	0.02%	0.003%
31	6.568	895	899	901	rBV	171	290	0.05%	0.006%
32	6.757	922	930	950	rBV	194205	473817	80.99%	9.709%
33	7.025	972	974	977	rBV2	179	195	0.03%	0.004%
34	7.123	984	990	995	rVB4	967	2185	0.37%	0.045%
35	7.214	1003	1005	1006	rBV2	416	380	0.06%	0.008%
36	7.306	1012	1020	1037	rBV	114679	265856	45.45%	5.448%

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Integrator: RTE

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

37	7.476	1047	1048	1049	rBV	221	107	0.02%	0.002%
38	7.787	1097	1099	1101	rVB2	175	113	0.02%	0.002%
39	7.952	1122	1126	1127	rBV	849	757	0.13%	0.016%
40	8.202	1165	1167	1170	rVB2	187	143	0.02%	0.003%
41	8.244	1170	1174	1175	rBV2	156	235	0.04%	0.005%
42	8.324	1181	1187	1202	rBV	61597	110577	18.90%	2.266%
43	8.592	1228	1231	1232	rBV2	120	113	0.02%	0.002%
44	8.647	1234	1240	1250	rBV	296813	462841	79.12%	9.484%
45	8.915	1280	1284	1285	rBV4	562	711	0.12%	0.015%
46	8.952	1285	1290	1300	rBV	46181	70083	11.98%	1.436%
47	9.275	1338	1343	1351	rVB2	8014	11958	2.04%	0.245%
48	9.391	1357	1362	1383	rBV	157219	326542	55.82%	6.691%
49	9.714	1411	1415	1423	rVB3	1285	2002	0.34%	0.041%
50	9.787	1425	1427	1429	rVB2	251	191	0.03%	0.004%
51	9.830	1432	1434	1435	rBV	163	121	0.02%	0.002%
52	9.890	1442	1444	1447	rVB2	161	161	0.03%	0.003%
53	9.915	1447	1448	1450	rBV	259	150	0.03%	0.003%
54	10.055	1465	1471	1483	rBV	403049	561732	96.02%	11.510%
55	10.311	1508	1513	1516	rBV2	999	1721	0.29%	0.035%
56	10.531	1547	1549	1551	rBV2	91	87	0.01%	0.002%
57	10.622	1562	1564	1565	rBV	120	92	0.02%	0.002%
58	10.646	1565	1568	1573	rVV2	416	589	0.10%	0.012%
59	10.829	1596	1598	1603	rVB2	102	116	0.02%	0.002%
60	10.878	1603	1606	1612	rBV4	508	926	0.16%	0.019%
61	10.970	1617	1621	1626	rBV2	1759	2495	0.43%	0.051%
62	11.043	1632	1633	1634	rBV	159	97	0.02%	0.002%
63	11.067	1634	1637	1639	rVV2	287	308	0.05%	0.006%
64	11.091	1639	1641	1647	rVB2	245	381	0.07%	0.008%
65	11.195	1652	1658	1669	rVV	246929	327195	55.93%	6.704%
66	11.390	1688	1690	1692	rBV2	156	114	0.02%	0.002%
67	11.433	1694	1697	1702	rVV2	1767	2429	0.42%	0.050%
68	11.482	1702	1705	1713	rVB2	2055	3155	0.54%	0.065%
69	11.707	1740	1742	1743	rBV	216	162	0.03%	0.003%
70	11.762	1746	1751	1764	rBV	25853	45430	7.77%	0.931%
71	11.933	1776	1779	1783	rBV3	1345	1483	0.25%	0.030%
72	11.982	1783	1787	1789	rBV2	2557	3677	0.63%	0.075%
73	12.024	1789	1794	1805	rVB	416303	537961	91.96%	11.023%
74	12.225	1824	1827	1830	rBV2	897	1152	0.20%	0.024%
75	12.317	1837	1842	1850	rBV	332276	439373	75.11%	9.003%
76	12.597	1886	1888	1891	rBV2	545	507	0.09%	0.010%

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 Title : VOC Analysis

77	12.658	1896	1898	1900	rBV2	126	76	0.01%	0.002%
78	12.719	1906	1908	1910	rVB	207	158	0.03%	0.003%
79	12.762	1910	1915	1921	rBV3	966	1521	0.26%	0.031%
80	12.841	1926	1928	1929	rBV2	276	289	0.05%	0.006%
81	12.872	1929	1933	1945	rVB2	8382	12446	2.13%	0.255%
82	13.036	1957	1960	1962	rBV2	171	167	0.03%	0.003%
83	13.116	1970	1973	1975	rBV2	261	352	0.06%	0.007%
84	13.170	1977	1982	1985	rBV2	335	534	0.09%	0.011%
85	13.219	1989	1990	1995	rVB3	466	454	0.08%	0.009%
86	13.268	1995	1998	2002	rBV3	537	782	0.13%	0.016%
87	13.359	2011	2013	2014	rBV	175	101	0.02%	0.002%
88	13.408	2018	2021	2023	rVB2	706	776	0.13%	0.016%
89	13.530	2039	2041	2043	rBV	108	76	0.01%	0.002%
90	13.682	2063	2066	2071	rBV3	1271	1689	0.29%	0.035%
91	13.786	2078	2083	2087	rBV2	2258	3155	0.54%	0.065%
92	13.847	2089	2093	2094	rBV3	181	210	0.04%	0.004%
93	13.884	2097	2099	2103	rBV2	799	832	0.14%	0.017%
94	14.036	2122	2124	2127	rBV2	505	456	0.08%	0.009%
95	14.128	2135	2139	2143	rBV2	1498	2065	0.35%	0.042%
96	14.280	2162	2164	2168	rVB3	285	303	0.05%	0.006%
97	14.432	2185	2189	2196	rVB	1722	2375	0.41%	0.049%
98	14.560	2203	2210	2213	rBV4	858	1835	0.31%	0.038%
99	14.646	2221	2224	2229	rVB3	782	1055	0.18%	0.022%
100	15.176	2307	2311	2315	rBV4	1242	1669	0.29%	0.034%

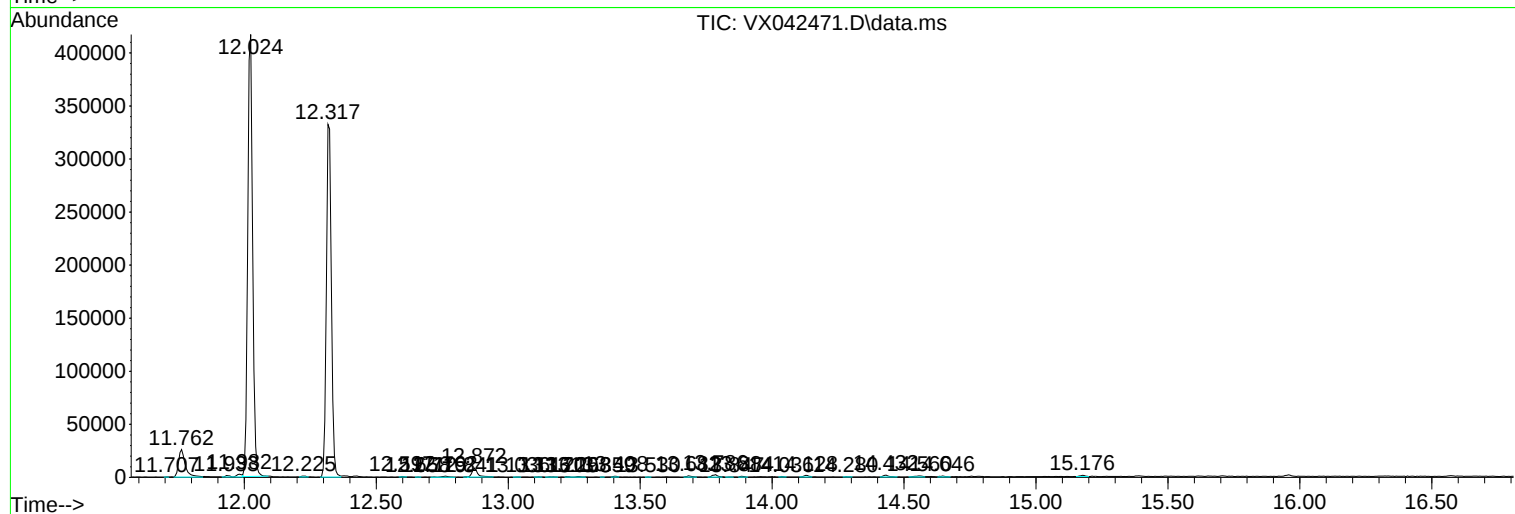
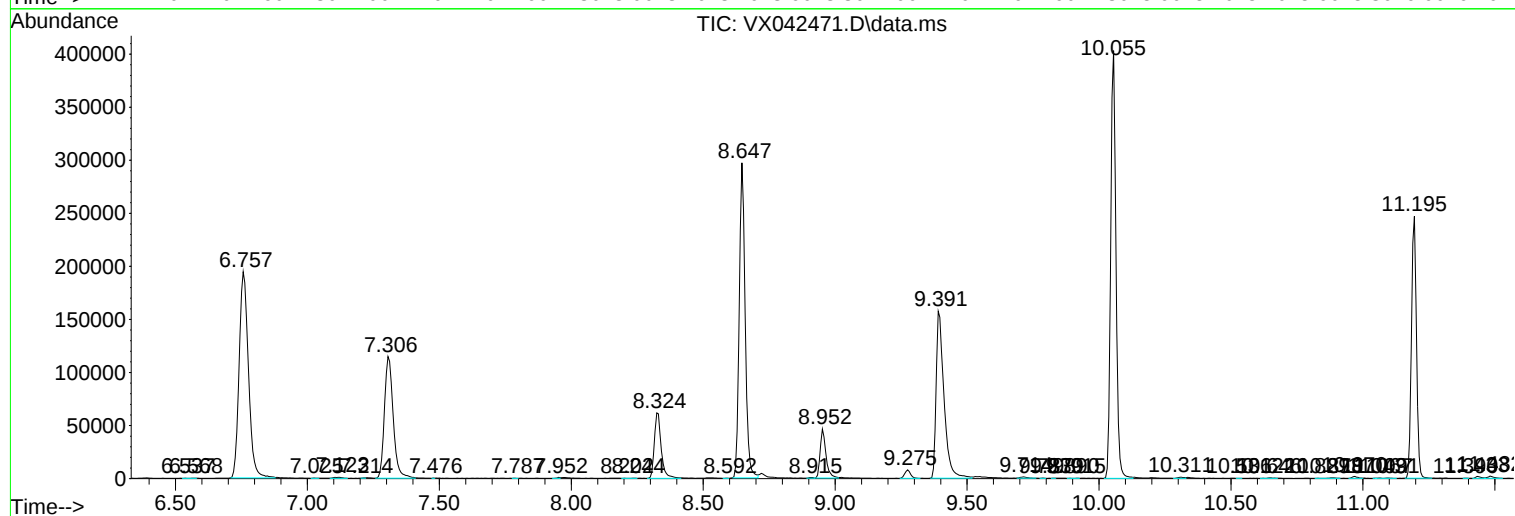
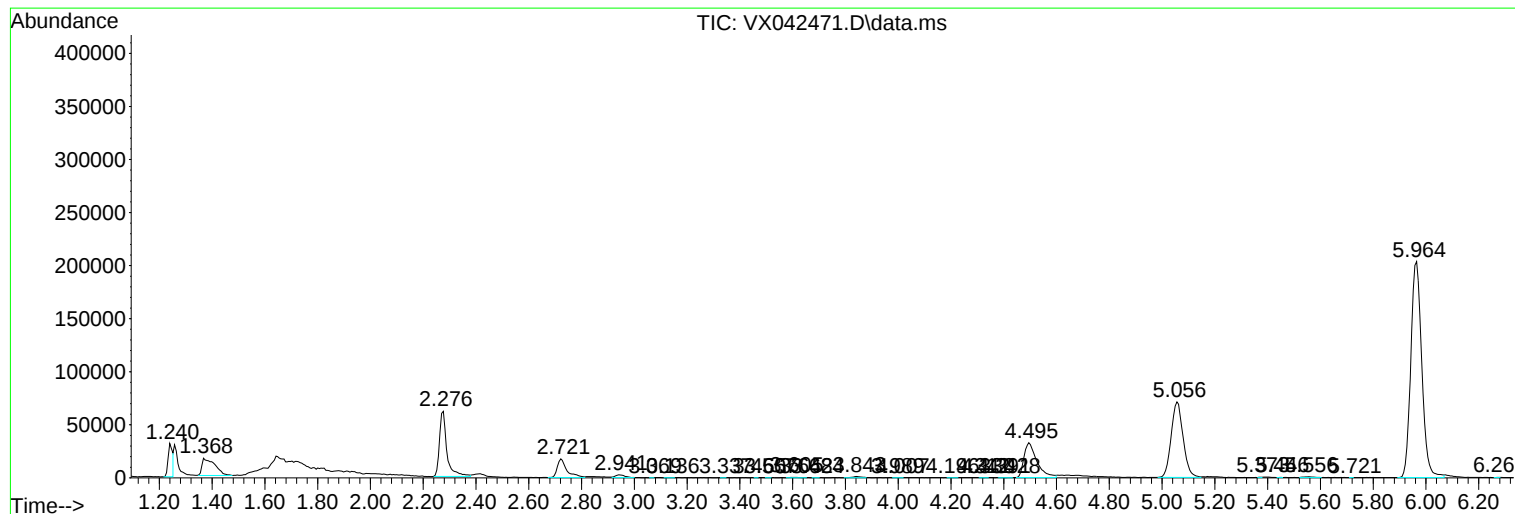
Sum of corrected areas: 4880309

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
A4CK3ME

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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Instrument :
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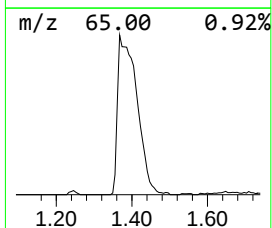
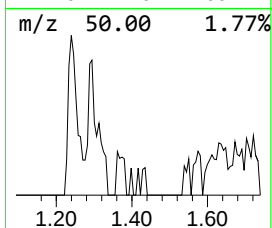
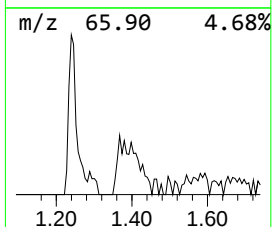
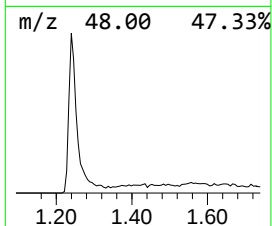
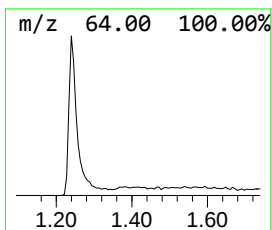
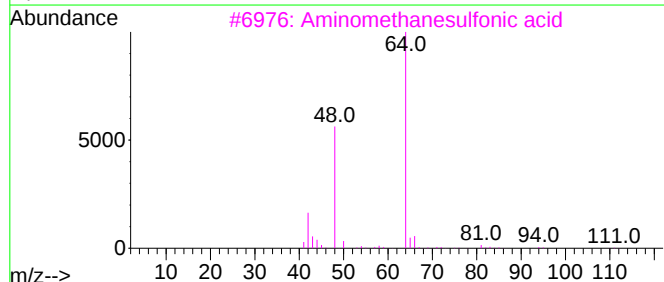
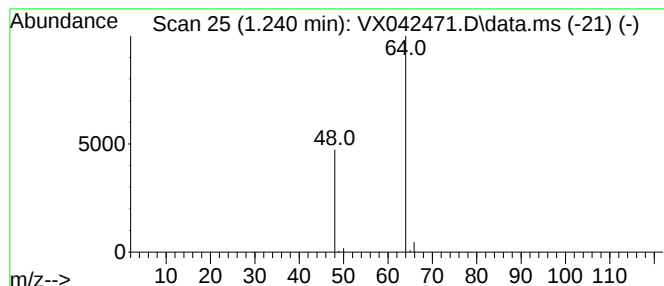
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM070324WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.95 ug/L	37476	1,4-Difluorobenzene	6.757

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	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	4



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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	4.0	ug/L	37476	1	6.757	473817	50.0