

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072024\
 Data File : VX042413.D
 Acq On : 19 Jul 2024 19:38
 Operator : JC/MD
 Sample : P3238-16ME
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BZ6ME

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: VX042413.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	21	25	27	rBV	38083	43470	7.99%	0.951%
2	1.367	43	46	64	rVB	36189	89318	16.42%	1.954%
3	1.642	89	91	108	rVB	20066	57908	10.65%	1.267%
4	2.282	189	196	211	rBV	88990	166250	30.56%	3.637%
5	2.532	235	237	240	rBV	227	236	0.04%	0.005%
6	2.715	262	267	274	rBV	3888	7775	1.43%	0.170%
7	2.782	274	278	285	rVB4	1625	3194	0.59%	0.070%
8	2.946	297	305	313	rBV	5492	14000	2.57%	0.306%
9	3.050	321	322	325	rVB	206	143	0.03%	0.003%
10	3.227	350	351	353	rBV	165	119	0.02%	0.003%
11	3.440	384	386	389	rBV2	97	117	0.02%	0.003%
12	3.611	412	414	419	rBB2	155	238	0.04%	0.005%
13	3.709	429	430	432	rBV	103	83	0.02%	0.002%
14	3.824	447	449	451	rBV2	110	117	0.02%	0.003%
15	3.922	463	465	467	rBV2	117	93	0.02%	0.002%
16	3.983	473	475	478	rBV	106	124	0.02%	0.003%
17	4.117	494	497	500	rBV	111	130	0.02%	0.003%
18	4.147	500	502	505	rVB2	134	127	0.02%	0.003%
19	4.336	531	533	535	rBV2	134	123	0.02%	0.003%
20	4.489	549	558	574	rBV2	28566	100774	18.52%	2.204%
21	4.928	628	630	632	rBV	154	139	0.03%	0.003%
22	5.056	640	651	671	rBV	67590	205107	37.70%	4.487%
23	5.239	680	681	684	rBV	187	199	0.04%	0.004%
24	5.385	701	705	706	rBV2	290	367	0.07%	0.008%
25	5.550	726	732	733	rBV2	325	489	0.09%	0.011%
26	5.635	745	746	749	rBV2	104	114	0.02%	0.002%
27	5.842	778	780	782	rBV	150	159	0.03%	0.003%
28	5.861	782	783	786	rBV2	107	92	0.02%	0.002%
29	5.964	789	800	817	rBV2	192422	543991	100.00%	11.900%
30	6.507	887	889	892	rBV	141	129	0.02%	0.003%
31	6.568	897	899	900	rVV2	151	94	0.02%	0.002%
32	6.586	900	902	903	rVB	240	160	0.03%	0.003%
33	6.610	903	906	909	rBV	166	239	0.04%	0.005%
34	6.653	911	913	915	rBV2	123	123	0.02%	0.003%
35	6.757	921	930	949	rBV	183288	446192	82.02%	9.760%
36	7.110	984	988	995	rVB4	947	1857	0.34%	0.041%

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 Title : VOC Analysis

37	7.202	1001	1003	1004	rBV	276	277	0.05%	0.006%
38	7.220	1004	1006	1011	rVB4	412	544	0.10%	0.012%
39	7.305	1012	1020	1037	rVV	106237	238601	43.86%	5.219%
40	7.470	1046	1047	1049	rBV2	244	212	0.04%	0.005%
41	7.629	1070	1073	1078	rBV2	119	220	0.04%	0.005%
42	7.702	1083	1085	1087	rVB	217	146	0.03%	0.003%
43	7.958	1124	1127	1131	rBV3	475	792	0.15%	0.017%
44	8.324	1181	1187	1199	rBV	60396	103432	19.01%	2.263%
45	8.464	1209	1210	1213	rVB2	158	104	0.02%	0.002%
46	8.525	1215	1220	1223	rBV2	586	984	0.18%	0.022%
47	8.647	1233	1240	1257	rBV	289924	459966	84.55%	10.062%
48	8.951	1285	1290	1306	rBV	43025	66655	12.25%	1.458%
49	9.110	1315	1316	1318	rBV	221	109	0.02%	0.002%
50	9.159	1320	1324	1326	rBV2	103	131	0.02%	0.003%
51	9.275	1340	1343	1347	rVB2	332	464	0.09%	0.010%
52	9.390	1357	1362	1378	rBV	125578	240120	44.14%	5.253%
53	9.646	1402	1404	1408	rVB2	230	273	0.05%	0.006%
54	9.714	1411	1415	1419	rVV3	1070	1464	0.27%	0.032%
55	9.829	1432	1434	1435	rBV	202	111	0.02%	0.002%
56	10.055	1465	1471	1489	rVV	380948	521013	95.78%	11.397%
57	10.232	1498	1500	1503	rVB2	178	179	0.03%	0.004%
58	10.256	1503	1504	1506	rBV2	122	102	0.02%	0.002%
59	10.281	1506	1508	1509	rVV	178	93	0.02%	0.002%
60	10.311	1509	1513	1522	rVB3	669	1054	0.19%	0.023%
61	10.604	1558	1561	1565	rBV	163	226	0.04%	0.005%
62	10.787	1589	1591	1594	rBV2	97	84	0.02%	0.002%
63	10.823	1594	1597	1598	rBV	117	102	0.02%	0.002%
64	10.969	1617	1621	1628	rVB2	738	1011	0.19%	0.022%
65	11.097	1638	1642	1643	rBV2	213	274	0.05%	0.006%
66	11.195	1652	1658	1666	rBV	208860	275969	50.73%	6.037%
67	11.311	1673	1677	1682	rBV	6777	9530	1.75%	0.208%
68	11.451	1698	1700	1703	rBV2	158	196	0.04%	0.004%
69	11.482	1703	1705	1707	rVB	318	243	0.04%	0.005%
70	11.616	1724	1727	1728	rBV	110	99	0.02%	0.002%
71	11.756	1744	1750	1754	rBV3	422	724	0.13%	0.016%
72	11.939	1779	1780	1782	rVB	154	87	0.02%	0.002%
73	12.024	1788	1794	1806	rBV	389447	511976	94.11%	11.199%
74	12.231	1824	1828	1829	rBV2	273	333	0.06%	0.007%
75	12.268	1832	1834	1837	rBV2	135	126	0.02%	0.003%
76	12.317	1837	1842	1855	rBV	316961	421318	77.45%	9.216%

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77	12.573	1882	1884	1886	rBV2	114	91	0.02%	0.002%
78	12.695	1900	1904	1906	rBV2	125	180	0.03%	0.004%
79	12.762	1910	1915	1921	rVB2	3630	5165	0.95%	0.113%
80	12.872	1927	1933	1940	rBV	2880	3933	0.72%	0.086%
81	13.030	1957	1959	1963	rBV3	205	325	0.06%	0.007%
82	13.103	1969	1971	1974	rBV2	110	127	0.02%	0.003%
83	13.189	1983	1985	1988	rBV2	159	213	0.04%	0.005%
84	13.323	2005	2007	2009	rBV	109	88	0.02%	0.002%
85	13.402	2017	2020	2026	rBV2	2097	3094	0.57%	0.068%
86	13.585	2049	2050	2056	rBV3	309	424	0.08%	0.009%
87	13.688	2063	2067	2070	rBV3	432	566	0.10%	0.012%
88	13.780	2079	2082	2087	rVB	1186	1850	0.34%	0.040%
89	13.823	2087	2089	2093	rVB2	207	269	0.05%	0.006%
90	13.890	2097	2100	2101	rBV2	150	127	0.02%	0.003%
91	13.963	2109	2112	2117	rBV3	272	429	0.08%	0.009%
92	14.005	2117	2119	2121	rBV2	214	227	0.04%	0.005%
93	14.127	2135	2139	2145	rBV2	2050	2988	0.55%	0.065%
94	14.383	2180	2181	2183	rBV2	230	173	0.03%	0.004%
95	14.432	2186	2189	2194	rVV3	1615	2002	0.37%	0.044%
96	14.615	2218	2219	2221	rBV2	280	193	0.04%	0.004%
97	14.652	2221	2225	2229	rVB4	523	873	0.16%	0.019%
98	14.774	2243	2245	2246	rBV2	444	265	0.05%	0.006%
99	14.889	2260	2264	2270	rBV2	1118	1757	0.32%	0.038%
100	15.956	2435	2439	2443	rBV2	1945	2957	0.54%	0.065%

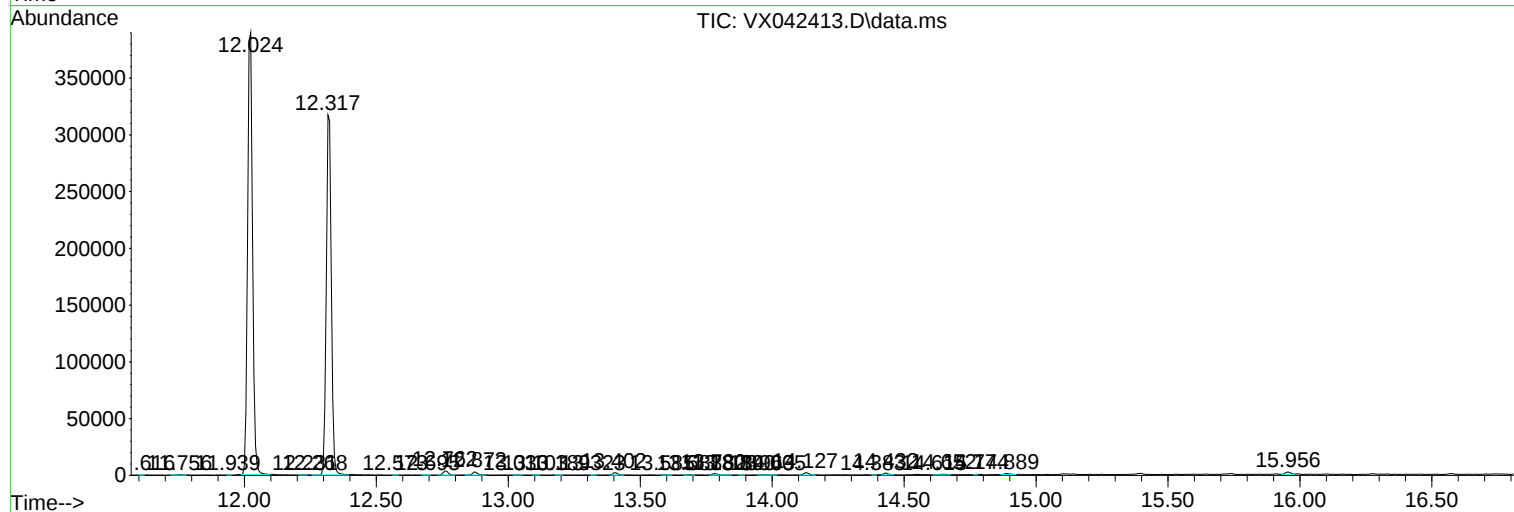
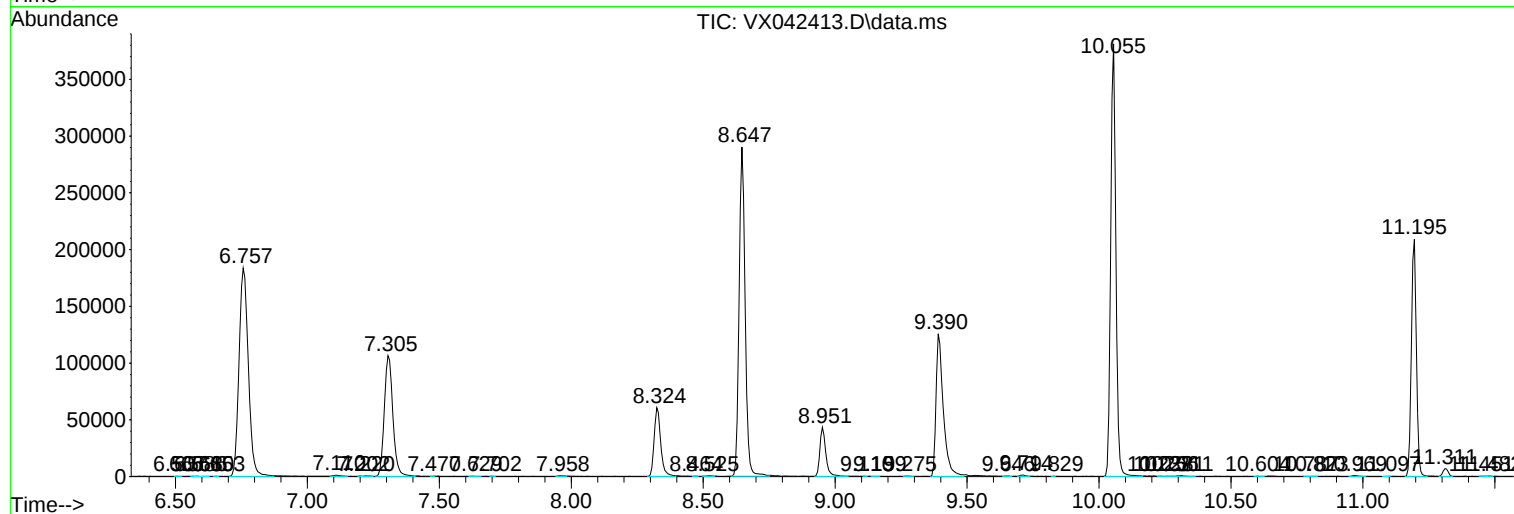
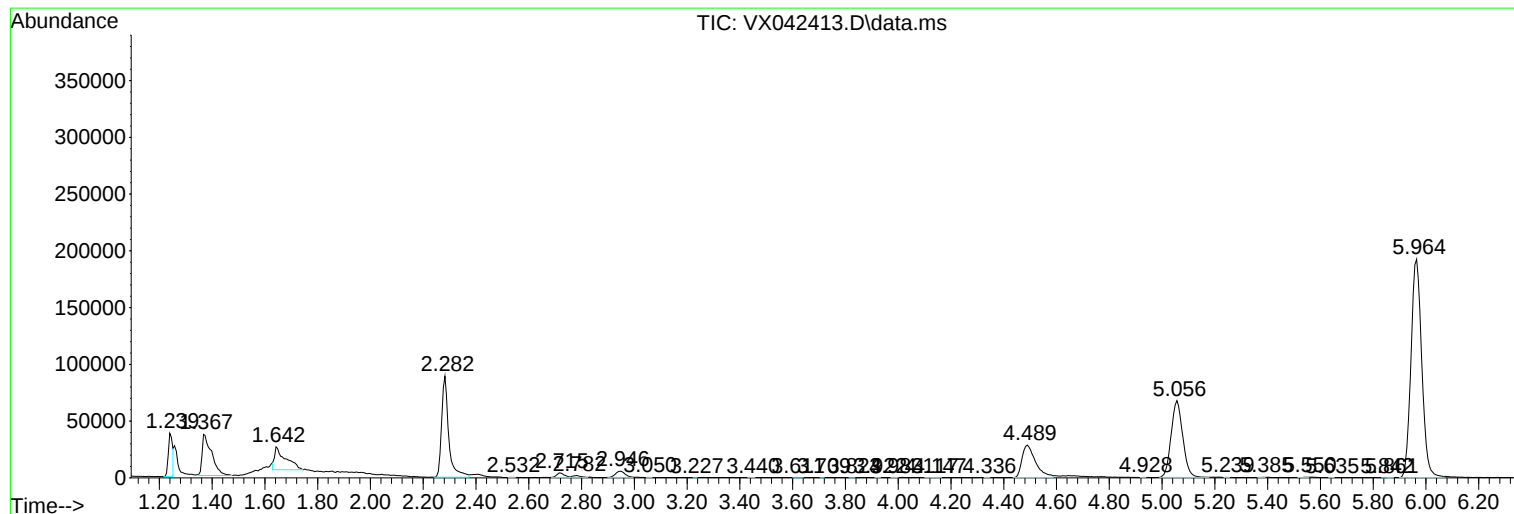
Sum of corrected areas: 4571450

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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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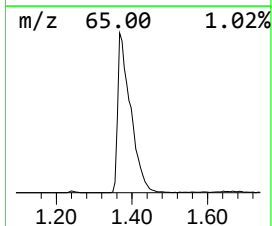
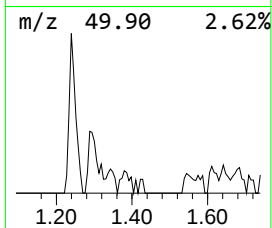
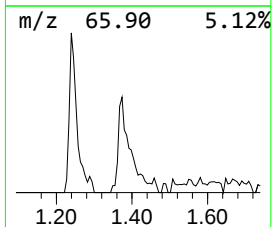
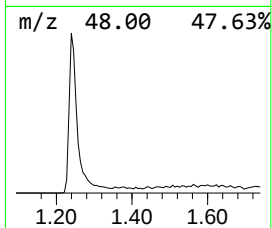
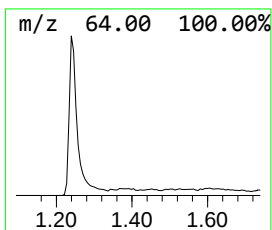
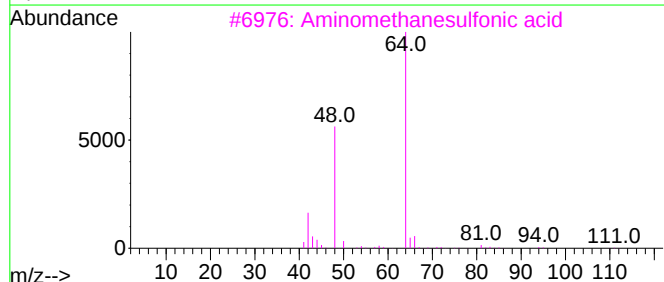
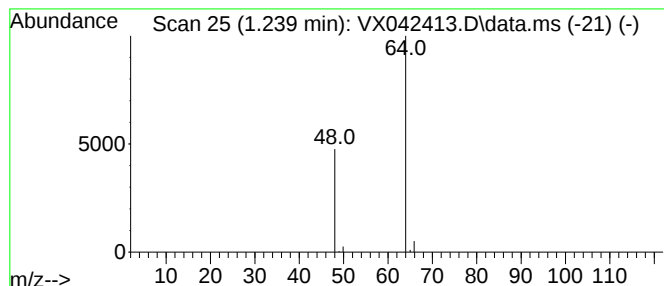
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	4.87 ug/L	43470	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	1.239	4.9	ug/L	43470	1	6.757	446192	50.0