

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042472.D
 Acq On : 23 Jul 2024 15:21
 Operator : JC/MD
 Sample : P3264-08ME
 Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BD8ME

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: VX042472.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	28835	34087	5.50%	0.680%
2	1.368	43	46	48	rBV	17498	22237	3.59%	0.444%
3	1.648	89	92	94	rBV	10998	14684	2.37%	0.293%
4	2.276	189	195	209	rBV	89443	169084	27.27%	3.372%
5	2.654	256	257	259	rBV2	295	240	0.04%	0.005%
6	2.721	265	268	273	rBV2	1031	1487	0.24%	0.030%
7	2.776	273	277	285	rVB2	1670	2955	0.48%	0.059%
8	2.947	298	305	316	rBV	2897	7239	1.17%	0.144%
9	3.020	316	317	321	rVB2	130	128	0.02%	0.003%
10	3.062	321	324	327	rBV2	120	140	0.02%	0.003%
11	3.099	327	330	333	rBV2	111	149	0.02%	0.003%
12	3.416	380	382	385	rVB2	222	259	0.04%	0.005%
13	3.532	400	401	403	rBV2	163	124	0.02%	0.002%
14	3.587	408	410	411	rBV	338	255	0.04%	0.005%
15	3.751	434	437	440	rBV	140	151	0.02%	0.003%
16	3.812	445	447	449	rVB2	147	128	0.02%	0.003%
17	3.861	454	455	457	rBV	143	99	0.02%	0.002%
18	3.910	460	463	466	rBV2	149	218	0.04%	0.004%
19	3.959	466	471	472	rBV	131	207	0.03%	0.004%
20	3.977	472	474	477	rBV2	96	111	0.02%	0.002%
21	4.062	487	488	491	rBV2	163	144	0.02%	0.003%
22	4.141	499	501	503	rVB2	121	105	0.02%	0.002%
23	4.276	521	523	525	rBV	123	109	0.02%	0.002%
24	4.355	533	536	537	rBV	110	109	0.02%	0.002%
25	4.495	547	559	577	rBV	38456	135295	21.82%	2.698%
26	5.050	640	650	668	rBV	75776	239681	38.66%	4.780%
27	5.306	690	692	697	rBV2	127	188	0.03%	0.004%
28	5.385	703	705	707	rBV	245	268	0.04%	0.005%
29	5.428	710	712	713	rBV2	119	103	0.02%	0.002%
30	5.544	726	731	733	rBV2	402	610	0.10%	0.012%
31	5.733	760	762	763	rBV2	164	127	0.02%	0.003%
32	5.849	780	781	785	rVB2	179	131	0.02%	0.003%
33	5.964	789	800	814	rBV2	216431	620036	100.00%	12.366%
34	6.190	835	837	840	rBV	158	117	0.02%	0.002%
35	6.391	867	870	876	rBV2	283	511	0.08%	0.010%
36	6.440	876	878	883	rVB	119	152	0.02%	0.003%

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Integration Parameters: LSCINT.P

Integrator: RTE

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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

37	6.495	883	887	888	rVB2	142	156	0.03%	0.003%
38	6.537	891	894	895	rBV2	107	96	0.02%	0.002%
39	6.757	921	930	958	rBV	203445	501272	80.85%	9.998%
40	7.117	983	989	995	rVB6	1134	2417	0.39%	0.048%
41	7.220	1001	1006	1012	rBV4	660	1663	0.27%	0.033%
42	7.306	1012	1020	1041	rVB	122909	279474	45.07%	5.574%
43	7.476	1046	1048	1049	rBV	219	189	0.03%	0.004%
44	7.653	1075	1077	1081	rVB2	177	169	0.03%	0.003%
45	7.824	1101	1105	1107	rVB2	119	146	0.02%	0.003%
46	7.958	1122	1127	1129	rBV4	643	1028	0.17%	0.021%
47	8.049	1141	1142	1144	rBV	129	121	0.02%	0.002%
48	8.324	1181	1187	1204	rBV	65289	117612	18.97%	2.346%
49	8.525	1215	1220	1221	rBV2	386	587	0.09%	0.012%
50	8.647	1234	1240	1256	rBV	315694	496773	80.12%	9.908%
51	8.952	1285	1290	1304	rBV	47067	74676	12.04%	1.489%
52	9.104	1313	1315	1318	rBV2	198	246	0.04%	0.005%
53	9.275	1337	1343	1351	rVB2	6606	10371	1.67%	0.207%
54	9.397	1357	1363	1386	rBV	147603	319537	51.54%	6.373%
55	9.647	1403	1404	1405	rVB	310	113	0.02%	0.002%
56	9.665	1405	1407	1410	rVB3	263	196	0.03%	0.004%
57	9.708	1411	1414	1422	rVB2	882	1338	0.22%	0.027%
58	9.805	1428	1430	1432	rBV	231	188	0.03%	0.004%
59	9.854	1436	1438	1440	rBV2	196	187	0.03%	0.004%
60	9.878	1440	1442	1443	rBV2	176	136	0.02%	0.003%
61	10.012	1461	1464	1465	rBV	105	116	0.02%	0.002%
62	10.055	1465	1471	1488	rBV	421870	583750	94.15%	11.643%
63	10.305	1510	1512	1518	rBV3	404	547	0.09%	0.011%
64	10.409	1527	1529	1531	rVB	213	132	0.02%	0.003%
65	10.524	1545	1548	1550	rBV	195	268	0.04%	0.005%
66	10.646	1565	1568	1571	rBV2	328	296	0.05%	0.006%
67	10.732	1580	1582	1587	rVB2	117	98	0.02%	0.002%
68	10.963	1618	1620	1624	rVV3	209	166	0.03%	0.003%
69	11.055	1632	1635	1638	rBV	163	157	0.03%	0.003%
70	11.116	1641	1645	1647	rBV	269	348	0.06%	0.007%
71	11.195	1652	1658	1666	rBV	261850	337472	54.43%	6.731%
72	11.311	1675	1677	1684	rVB2	911	1233	0.20%	0.025%
73	11.402	1690	1692	1694	rBV	187	193	0.03%	0.004%
74	11.707	1740	1742	1744	rVB	170	108	0.02%	0.002%
75	11.750	1744	1749	1755	rBV5	761	1470	0.24%	0.029%
76	11.896	1772	1773	1775	rBV	151	99	0.02%	0.002%

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 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4BD8ME

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

77	11.933	1777	1779	1782	rVB	467	404	0.07%	0.008%
78	11.975	1785	1786	1788	rVB	298	156	0.03%	0.003%
79	12.024	1788	1794	1807	rBV	425347	550362	88.76%	10.977%
80	12.225	1825	1827	1829	rBV2	205	134	0.02%	0.003%
81	12.323	1837	1843	1858	rBV	343973	465532	75.08%	9.285%
82	12.488	1868	1870	1874	rVB2	220	197	0.03%	0.004%
83	12.652	1894	1897	1899	rBV2	107	104	0.02%	0.002%
84	12.670	1899	1900	1903	rBV2	135	108	0.02%	0.002%
85	12.762	1911	1915	1920	rVB2	845	1054	0.17%	0.021%
86	12.939	1942	1944	1951	rBV2	208	285	0.05%	0.006%
87	12.994	1951	1953	1954	rVV2	150	114	0.02%	0.002%
88	13.042	1957	1961	1965	rBV2	201	312	0.05%	0.006%
89	13.353	2010	2012	2014	rVV	145	96	0.02%	0.002%
90	13.530	2040	2041	2043	rBV2	180	112	0.02%	0.002%
91	13.670	2062	2064	2067	rBV2	247	273	0.04%	0.005%
92	13.786	2079	2083	2090	rVB3	822	1388	0.22%	0.028%
93	13.963	2110	2112	2117	rVB2	385	441	0.07%	0.009%
94	14.006	2117	2119	2122	rBV2	198	230	0.04%	0.005%
95	14.085	2131	2132	2134	rBV	202	162	0.03%	0.003%
96	14.134	2136	2140	2145	rVB2	1020	1574	0.25%	0.031%
97	14.329	2171	2172	2175	rBV	217	166	0.03%	0.003%
98	14.505	2200	2201	2202	rBV	202	96	0.02%	0.002%
99	14.554	2204	2209	2217	rVB6	1249	3488	0.56%	0.070%
100	14.780	2245	2246	2249	rBV	261	251	0.04%	0.005%

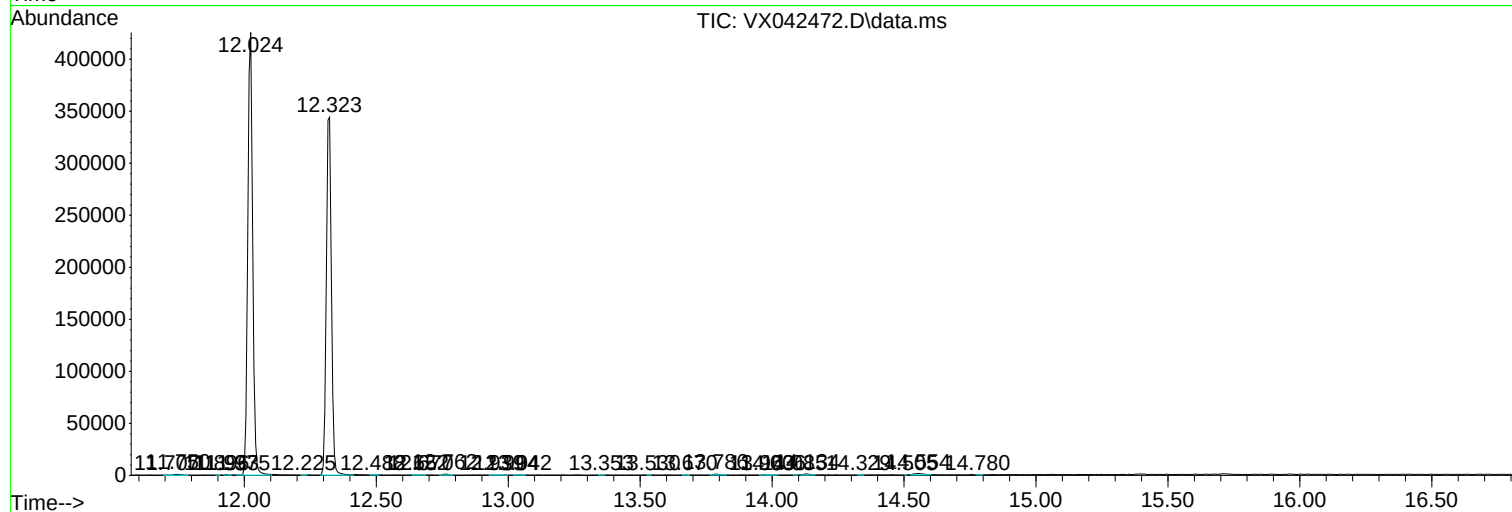
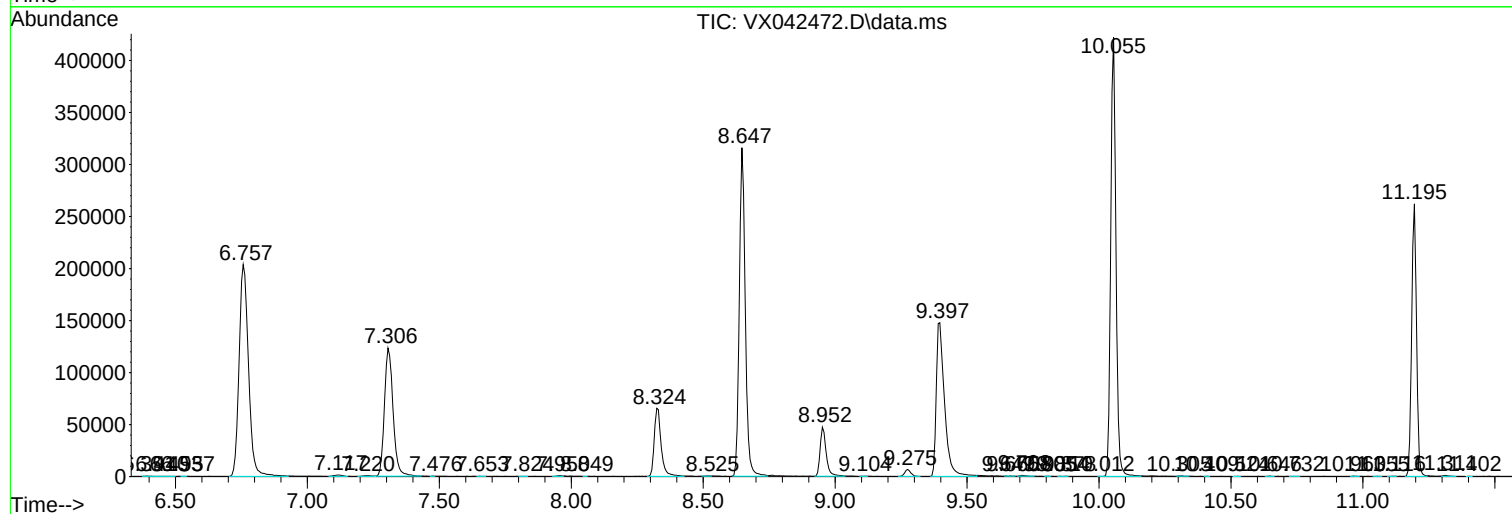
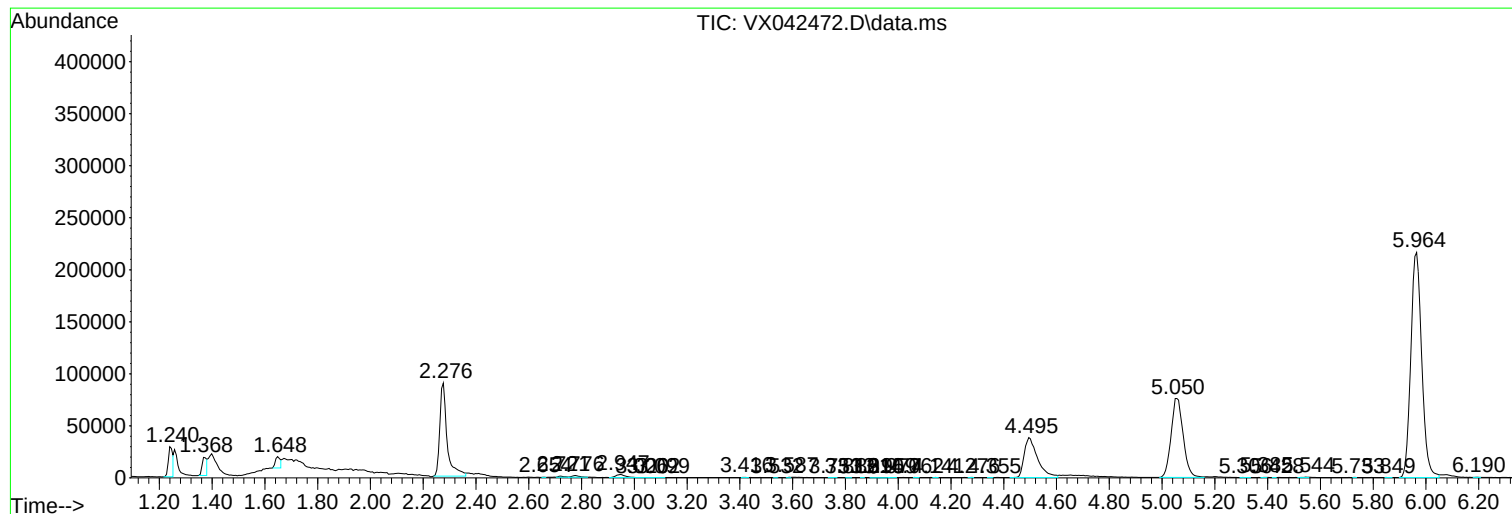
Sum of corrected areas: 5013851

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Sample : P3264-08ME
Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4BD8ME

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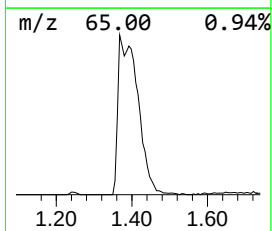
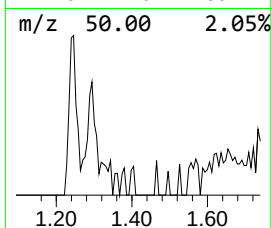
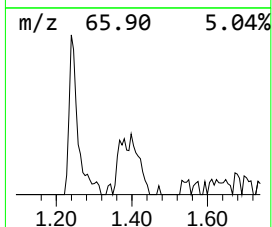
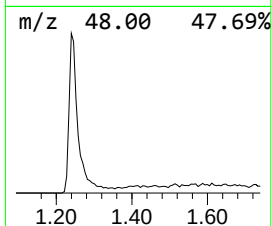
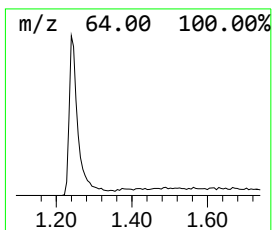
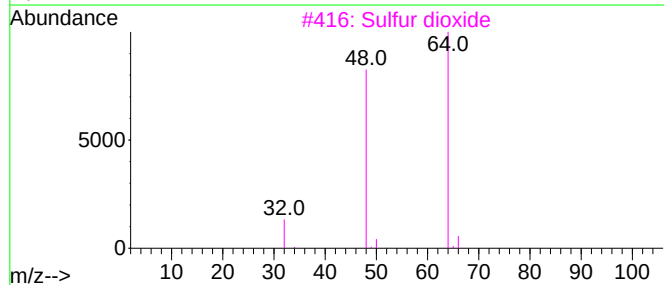
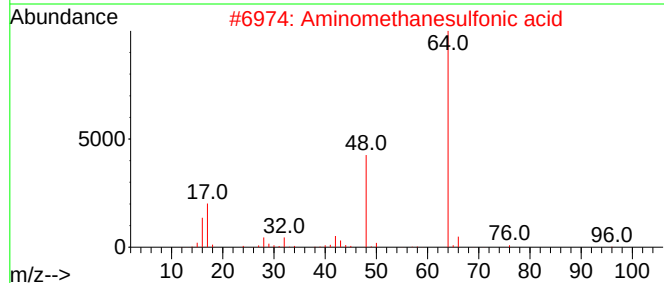
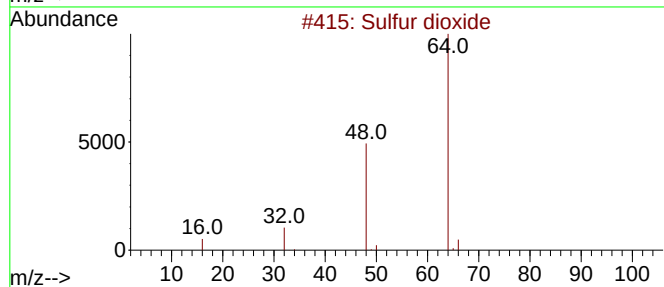
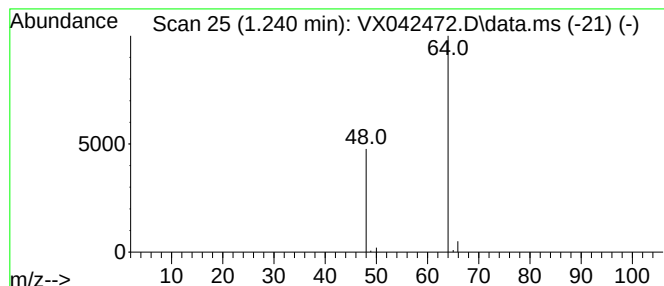
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.40 ug/L	34087	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			Sulfur dioxide	64	O2S	007446-09-5	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.4	ug/L	34087	1	6.757	501272	50.0