

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042484.D
 Acq On : 23 Jul 2024 20:00
 Operator : JC/MD
 Sample : P3327-15
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZX0

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: VX042484.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	7	9	16	rVB2	2663	3082	0.05%	0.026%
2	1.239	22	25	33	rBV	21981	30153	0.46%	0.251%
3	1.373	43	47	65	rVB2	446157	551337	8.45%	4.589%
4	1.648	88	92	101	rVB	50497	66433	1.02%	0.553%
5	2.087	160	164	171	rBV	6968	9896	0.15%	0.082%
6	2.300	192	199	210	rBV	133990	223657	3.43%	1.861%
7	2.568	238	243	250	rVB2	1260	2386	0.04%	0.020%
8	2.696	261	264	265	rBV2	174	145	0.00%	0.001%
9	2.715	265	267	271	rVV3	231	285	0.00%	0.002%
10	2.788	274	279	287	rVB5	891	2044	0.03%	0.017%
11	2.946	298	305	311	rVV2	1459	3522	0.05%	0.029%
12	3.019	315	317	319	rBV2	118	98	0.00%	0.001%
13	3.086	322	328	337	rVV3	2851	5804	0.09%	0.048%
14	3.166	339	341	342	rVB	105	60	0.00%	0.000%
15	3.184	342	344	346	rBV	146	119	0.00%	0.001%
16	3.269	357	358	359	rBV	118	75	0.00%	0.001%
17	3.367	373	374	376	rBV2	76	78	0.00%	0.001%
18	3.416	381	382	383	rBV	92	61	0.00%	0.001%
19	3.458	388	389	390	rBV	123	60	0.00%	0.000%
20	3.477	390	392	395	rBV2	101	110	0.00%	0.001%
21	3.507	395	397	400	rBV	112	164	0.00%	0.001%
22	3.611	405	414	425	rVV	14183	33237	0.51%	0.277%
23	3.684	425	426	432	rVB2	283	257	0.00%	0.002%
24	3.739	432	435	436	rBV	76	71	0.00%	0.001%
25	3.757	436	438	442	rVB2	88	105	0.00%	0.001%
26	3.836	449	451	454	rBV2	149	198	0.00%	0.002%
27	3.989	474	476	478	rBV2	94	93	0.00%	0.001%
28	4.251	518	519	522	rBV2	95	87	0.00%	0.001%
29	4.489	545	558	588	rBV	2357221	6524586	100.00%	54.303%
30	4.958	633	635	636	rBV	240	156	0.00%	0.001%
31	5.062	640	652	673	rVB	90191	270641	4.15%	2.252%
32	5.324	692	695	697	rBV2	102	114	0.00%	0.001%
33	5.391	703	706	707	rBV2	267	249	0.00%	0.002%
34	5.836	777	779	780	rBV	134	94	0.00%	0.001%
35	5.970	789	801	818	rBV2	230017	683213	10.47%	5.686%
36	6.354	862	864	865	rBV	127	95	0.00%	0.001%

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 Title : VOC Analysis

37	6.519	889	891	893	rBV2	99	99	0.00%	0.001%
38	6.659	912	914	915	rBV	111	73	0.00%	0.001%
39	6.763	922	931	947	rBV	182481	440475	6.75%	3.666%
40	7.013	971	972	975	rVB	180	107	0.00%	0.001%
41	7.128	984	991	1001	rVB4	4932	11768	0.18%	0.098%
42	7.214	1003	1005	1008	rVB3	320	306	0.00%	0.003%
43	7.311	1012	1021	1039	rBV	136061	303916	4.66%	2.529%
44	7.519	1053	1055	1056	rBV	149	93	0.00%	0.001%
45	7.567	1061	1063	1066	rBV2	87	106	0.00%	0.001%
46	7.714	1085	1087	1089	rBV	133	79	0.00%	0.001%
47	7.823	1102	1105	1106	rBV2	137	116	0.00%	0.001%
48	7.964	1123	1128	1132	rBV2	398	754	0.01%	0.006%
49	8.110	1150	1152	1158	rBV2	124	216	0.00%	0.002%
50	8.171	1160	1162	1166	rBV2	129	149	0.00%	0.001%
51	8.323	1181	1187	1206	rBV	79451	135900	2.08%	1.131%
52	8.518	1216	1219	1220	rBV	507	375	0.01%	0.003%
53	8.646	1234	1240	1261	rBV	344080	554339	8.50%	4.614%
54	8.951	1285	1290	1305	rBV	56782	86115	1.32%	0.717%
55	9.140	1319	1321	1324	rBV2	105	123	0.00%	0.001%
56	9.274	1339	1343	1348	rVB2	3423	5389	0.08%	0.045%
57	9.335	1351	1353	1356	rVB2	86	85	0.00%	0.001%
58	9.384	1356	1361	1379	rBV	200960	313054	4.80%	2.605%
59	9.756	1420	1422	1424	rVB2	181	131	0.00%	0.001%
60	9.780	1424	1426	1427	rBV2	146	112	0.00%	0.001%
61	10.012	1463	1464	1465	rBV	165	69	0.00%	0.001%
62	10.055	1465	1471	1485	rBV	372300	499397	7.65%	4.156%
63	10.231	1498	1500	1501	rVB	186	97	0.00%	0.001%
64	10.256	1501	1504	1505	rBV	192	147	0.00%	0.001%
65	10.359	1520	1521	1523	rBV	159	107	0.00%	0.001%
66	10.573	1554	1556	1558	rVB	169	116	0.00%	0.001%
67	10.597	1558	1560	1563	rBV2	111	120	0.00%	0.001%
68	10.622	1563	1564	1566	rBV	138	83	0.00%	0.001%
69	10.646	1566	1568	1571	rVV2	303	266	0.00%	0.002%
70	10.744	1582	1584	1587	rVB	148	96	0.00%	0.001%
71	10.774	1587	1589	1592	rBV2	104	102	0.00%	0.001%
72	10.939	1614	1616	1618	rBV2	123	84	0.00%	0.001%
73	10.969	1618	1621	1625	rBV2	194	251	0.00%	0.002%
74	11.073	1636	1638	1639	rBV	88	86	0.00%	0.001%
75	11.122	1644	1646	1647	rBV	146	136	0.00%	0.001%
76	11.195	1652	1658	1672	rBV	253359	340207	5.21%	2.831%

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77	11.439	1695	1698	1699	rBV	155	198	0.00%	0.002%
78	11.731	1743	1746	1747	rBV2	88	96	0.00%	0.001%
79	11.756	1747	1750	1753	rVB2	290	384	0.01%	0.003%
80	11.786	1753	1755	1758	rVB2	129	134	0.00%	0.001%
81	11.823	1758	1761	1762	rBV2	129	152	0.00%	0.001%
82	11.908	1773	1775	1777	rVB2	108	89	0.00%	0.001%
83	11.975	1784	1786	1788	rBV2	157	130	0.00%	0.001%
84	12.024	1788	1794	1809	rVV	328836	435645	6.68%	3.626%
85	12.219	1823	1826	1831	rBV2	3167	4145	0.06%	0.034%
86	12.316	1837	1842	1855	rBV	358827	463654	7.11%	3.859%
87	12.426	1859	1860	1863	rBV3	268	183	0.00%	0.002%
88	12.512	1872	1874	1876	rVB	253	163	0.00%	0.001%
89	13.194	1984	1986	1988	rBV	93	84	0.00%	0.001%
90	13.383	2016	2017	2021	rVV	153	157	0.00%	0.001%
91	13.450	2025	2028	2031	rBV	111	137	0.00%	0.001%
92	13.481	2031	2033	2037	rBB2	160	191	0.00%	0.002%
93	13.554	2043	2045	2046	rBV	108	70	0.00%	0.001%
94	13.859	2093	2095	2100	rVB2	117	164	0.00%	0.001%
95	13.975	2113	2114	2115	rVB	195	71	0.00%	0.001%
96	13.993	2115	2117	2119	rVB	222	151	0.00%	0.001%
97	14.030	2119	2123	2124	rBV2	150	136	0.00%	0.001%
98	14.127	2136	2139	2143	rVB	573	797	0.01%	0.007%
99	14.182	2146	2148	2149	rBV	134	87	0.00%	0.001%
100	14.255	2158	2160	2163	rBV2	171	209	0.00%	0.002%

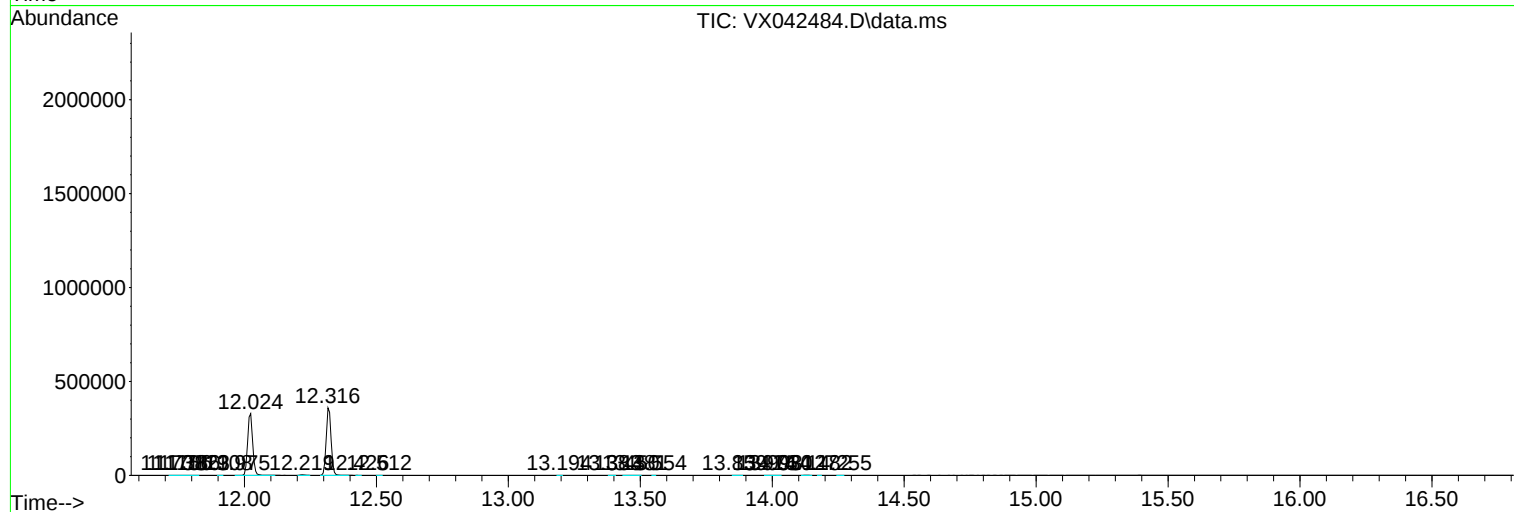
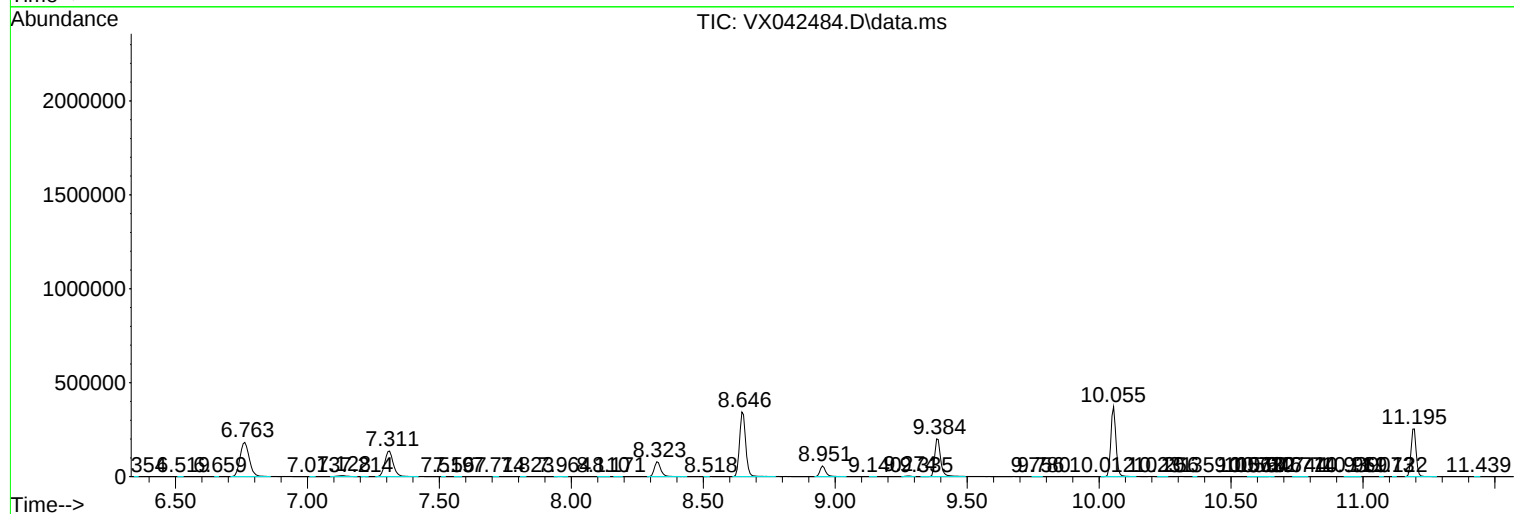
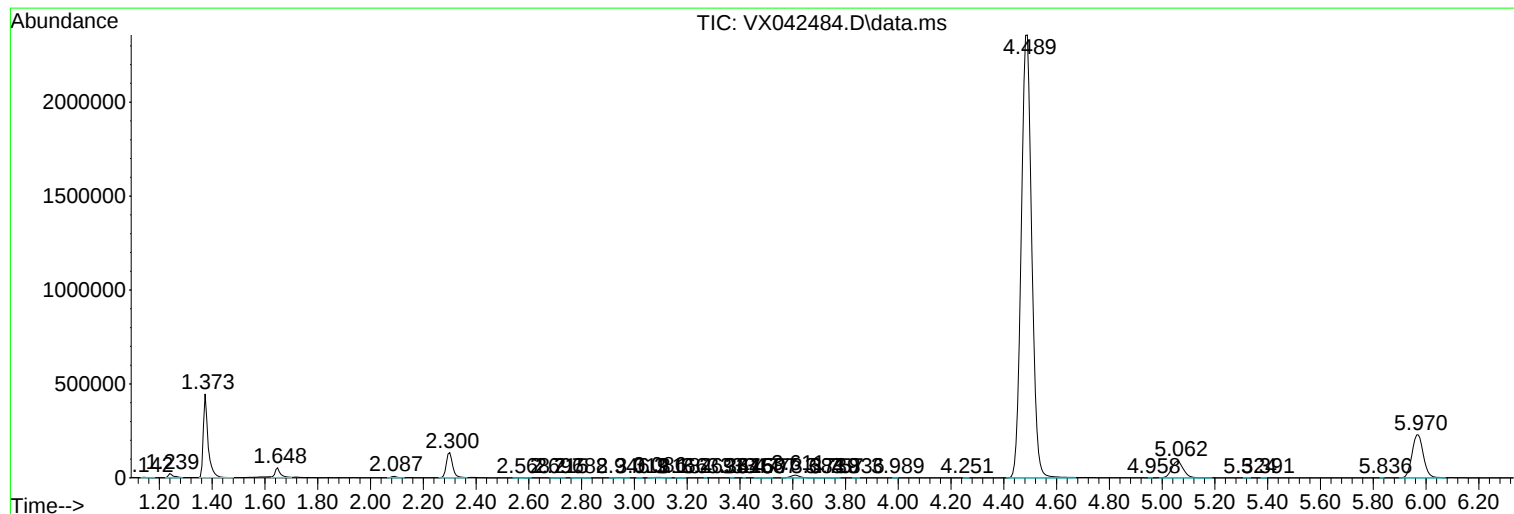
Sum of corrected areas: 12015236

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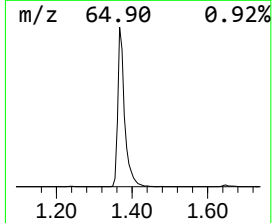
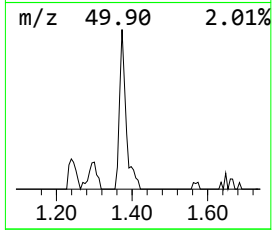
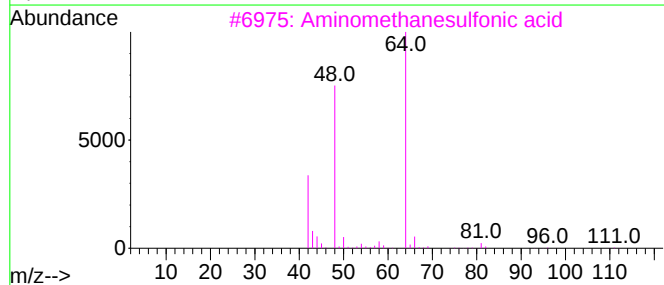
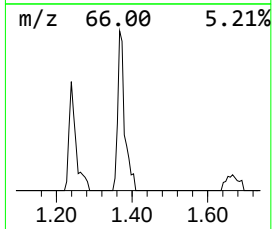
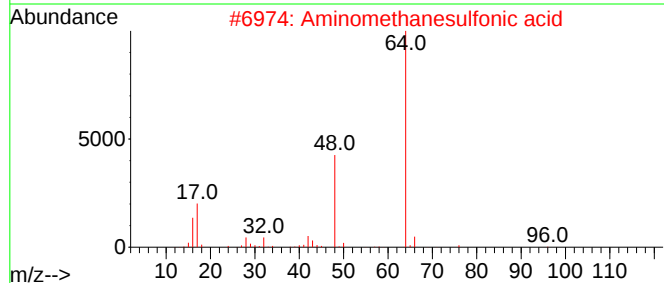
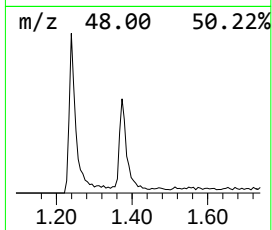
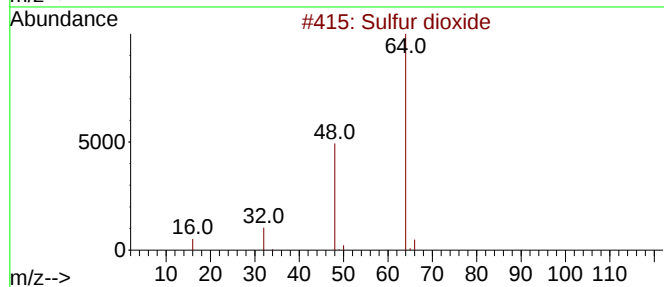
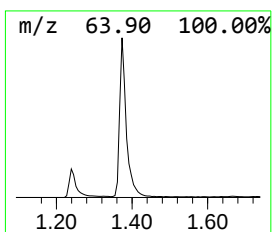
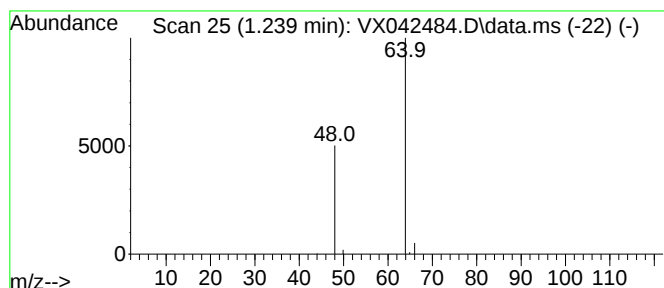
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	3.42 ug/L	30153	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 Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.239	3.4	ug/L	30153	1	6.763	440475	50.0