

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042482.D
 Acq On : 23 Jul 2024 19:13
 Operator : JC/MD
 Sample : P3327-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E1ZW8

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: VX042482.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	6	9	21	rVB	14423	18374	2.74%	0.367%
2	1.240	22	25	28	rBV	25786	28941	4.32%	0.578%
3	1.368	42	46	57	rVB	68362	84934	12.68%	1.696%
4	1.648	88	92	100	rVB	46505	62242	9.29%	1.243%
5	1.721	101	104	113	rVB4	7360	11755	1.75%	0.235%
6	1.935	136	139	145	rVB5	3056	4485	0.67%	0.090%
7	2.179	177	179	184	rVB2	272	258	0.04%	0.005%
8	2.294	192	198	208	rBV	128361	203780	30.42%	4.069%
9	2.386	210	213	225	rVB3	2765	5957	0.89%	0.119%
10	2.563	238	242	250	rVB	2228	3727	0.56%	0.074%
11	2.788	274	279	280	rBV2	942	1313	0.20%	0.026%
12	2.898	295	297	298	rVB	138	97	0.01%	0.002%
13	2.947	298	305	316	rBV2	2448	6363	0.95%	0.127%
14	3.087	325	328	334	rVB3	490	991	0.15%	0.020%
15	3.136	334	336	337	rBV	97	61	0.01%	0.001%
16	3.245	353	354	357	rVB2	158	131	0.02%	0.003%
17	3.270	357	358	359	rBV	110	72	0.01%	0.001%
18	3.331	367	368	372	rBV3	236	296	0.04%	0.006%
19	3.440	381	386	391	rVB3	598	1269	0.19%	0.025%
20	3.483	391	393	394	rBV2	132	112	0.02%	0.002%
21	3.562	404	406	409	rBV2	168	199	0.03%	0.004%
22	3.703	427	429	431	rBV2	93	102	0.02%	0.002%
23	3.770	438	440	441	rBV	87	62	0.01%	0.001%
24	3.825	448	449	450	rVB	109	40	0.01%	0.001%
25	3.886	455	459	461	rBV2	148	211	0.03%	0.004%
26	3.904	461	462	463	rBV	65	32	0.00%	0.001%
27	4.117	493	497	498	rBV	139	153	0.02%	0.003%
28	4.294	521	526	527	rBV3	524	777	0.12%	0.016%
29	4.471	546	555	572	rBV	49825	155025	23.14%	3.095%
30	4.971	633	637	638	rVB	224	155	0.02%	0.003%
31	5.056	638	651	669	rBV	85818	265850	39.68%	5.308%
32	5.251	681	683	684	rBV2	144	105	0.02%	0.002%
33	5.465	712	718	720	rBV4	613	1204	0.18%	0.024%
34	5.605	739	741	743	rBV2	131	125	0.02%	0.002%
35	5.788	769	771	774	rBV2	127	165	0.02%	0.003%
36	5.836	777	779	781	rBV	120	74	0.01%	0.001%

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

37	5.867	783	784	787	rBV	90	70	0.01%	0.001%
38	5.971	789	801	822	rBV2	224241	669901	100.00%	13.376%
39	6.349	861	863	866	rBV	227	231	0.03%	0.005%
40	6.531	890	893	895	rBV2	131	109	0.02%	0.002%
41	6.647	908	912	914	rBV2	171	267	0.04%	0.005%
42	6.763	922	931	948	rBV	171547	411130	61.37%	8.209%
43	7.074	980	982	984	rBV	218	244	0.04%	0.005%
44	7.129	984	991	1002	rVV	21449	48956	7.31%	0.978%
45	7.306	1012	1020	1039	rBV	132948	303841	45.36%	6.067%
46	7.775	1096	1097	1099	rBV	106	65	0.01%	0.001%
47	7.830	1105	1106	1108	rBV	142	90	0.01%	0.002%
48	7.964	1123	1128	1131	rBV2	406	637	0.10%	0.013%
49	8.056	1141	1143	1147	rVB2	159	166	0.02%	0.003%
50	8.086	1147	1148	1150	rBV	121	78	0.01%	0.002%
51	8.159	1158	1160	1164	rBV2	113	169	0.03%	0.003%
52	8.324	1181	1187	1204	rBV	74793	132780	19.82%	2.651%
53	8.513	1214	1218	1220	rBV2	363	496	0.07%	0.010%
54	8.647	1234	1240	1249	rBV	325345	519649	77.57%	10.376%
55	8.952	1285	1290	1301	rBV	56799	84799	12.66%	1.693%
56	9.171	1324	1326	1328	rBV	129	139	0.02%	0.003%
57	9.275	1339	1343	1352	rVB2	3250	5300	0.79%	0.106%
58	9.385	1356	1361	1384	rBV	206139	317407	47.38%	6.338%
59	9.805	1428	1430	1433	rBV3	151	184	0.03%	0.004%
60	9.884	1441	1443	1445	rBV2	126	122	0.02%	0.002%
61	10.012	1462	1464	1465	rBV	98	96	0.01%	0.002%
62	10.055	1465	1471	1490	rVV	334903	462132	68.99%	9.228%
63	10.201	1492	1495	1501	rVB	1355	1838	0.27%	0.037%
64	10.305	1508	1512	1521	rVB	2353	3413	0.51%	0.068%
65	10.586	1556	1558	1559	rVB2	149	99	0.01%	0.002%
66	10.640	1565	1567	1573	rVB2	1072	1446	0.22%	0.029%
67	10.695	1575	1576	1577	rVB	101	37	0.01%	0.001%
68	10.744	1582	1584	1586	rVV	150	106	0.02%	0.002%
69	10.768	1586	1588	1589	rVV	142	75	0.01%	0.001%
70	10.787	1589	1591	1594	rVB	121	78	0.01%	0.002%
71	11.189	1652	1657	1666	rBV	257679	343485	51.27%	6.859%
72	11.299	1673	1675	1677	rBV2	236	207	0.03%	0.004%
73	11.396	1686	1691	1693	rBV2	350	536	0.08%	0.011%
74	11.457	1697	1701	1705	rBV3	456	851	0.13%	0.017%
75	11.610	1723	1726	1727	rBV2	166	176	0.03%	0.004%
76	11.726	1743	1745	1747	rBV	135	97	0.01%	0.002%

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77	11.756	1747	1750	1754	rVV	1353	1354	0.20%	0.027%
78	11.817	1758	1760	1763	rBV2	103	108	0.02%	0.002%
79	11.927	1776	1778	1780	rVB	153	92	0.01%	0.002%
80	11.951	1780	1782	1783	rBV	117	80	0.01%	0.002%
81	11.976	1784	1786	1788	rVB	261	144	0.02%	0.003%
82	12.024	1788	1794	1803	rBV	298575	392172	58.54%	7.831%
83	12.219	1823	1826	1833	rVB2	4814	6094	0.91%	0.122%
84	12.317	1837	1842	1853	rBV	337434	434914	64.92%	8.684%
85	12.725	1908	1909	1910	rBV	136	79	0.01%	0.002%
86	12.756	1913	1914	1918	rVB2	201	210	0.03%	0.004%
87	12.963	1946	1948	1952	rVB3	208	253	0.04%	0.005%
88	13.000	1952	1954	1955	rVB	140	60	0.01%	0.001%
89	13.262	1996	1997	1998	rBV	157	72	0.01%	0.001%
90	13.292	1998	2002	2005	rVB2	203	257	0.04%	0.005%
91	13.609	2052	2054	2056	rVB2	174	117	0.02%	0.002%
92	13.786	2080	2083	2090	rVB4	336	556	0.08%	0.011%
93	13.878	2096	2098	2099	rBV2	147	103	0.02%	0.002%
94	14.231	2154	2156	2159	rBV	194	217	0.03%	0.004%
95	14.329	2170	2172	2174	rBV2	140	127	0.02%	0.003%
96	15.005	2281	2283	2285	rBV2	310	197	0.03%	0.004%

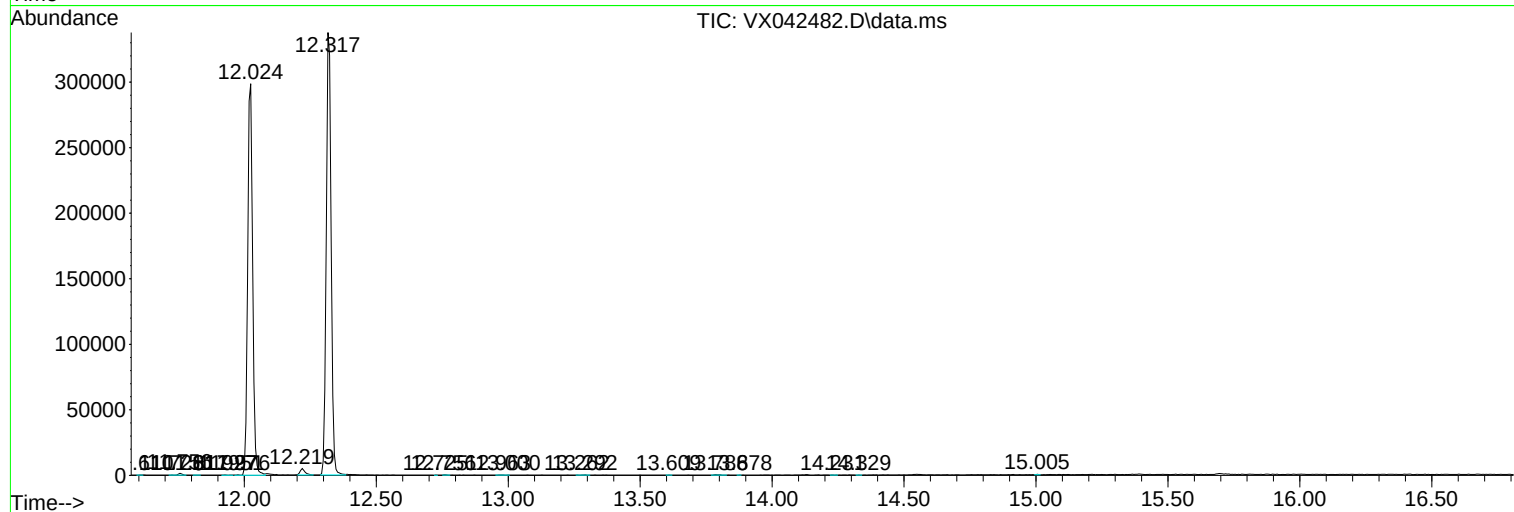
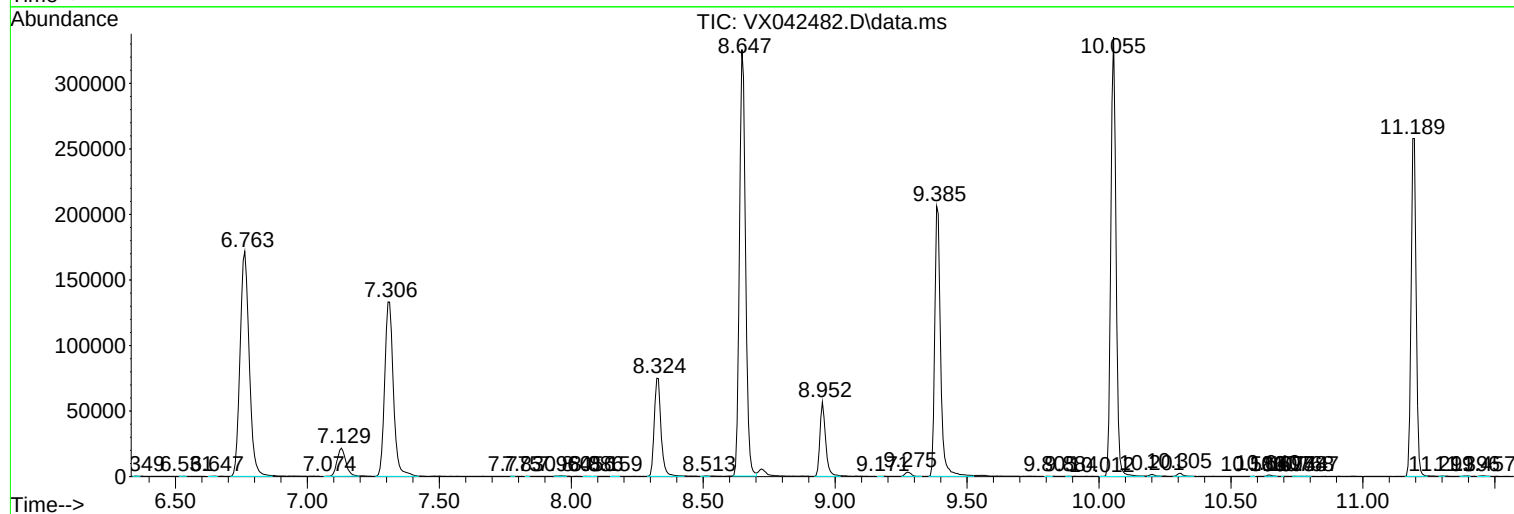
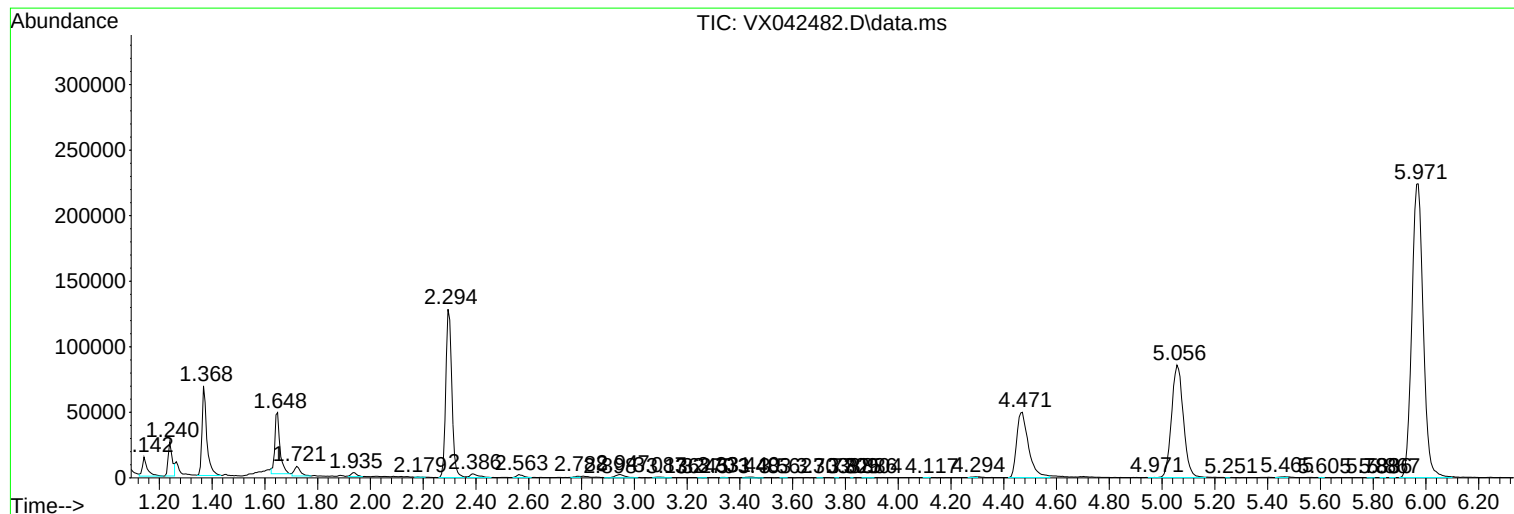
Sum of corrected areas: 5008145

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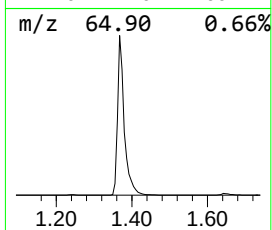
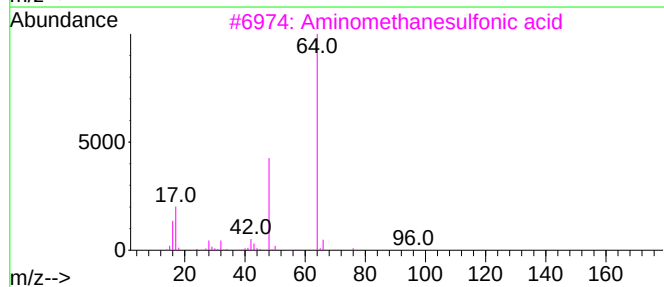
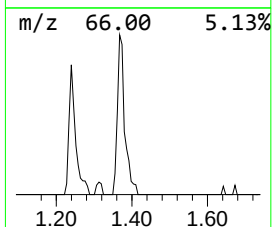
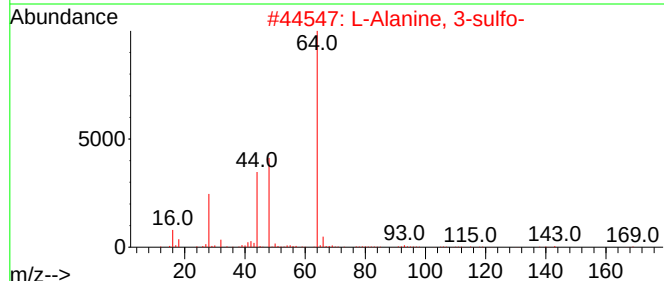
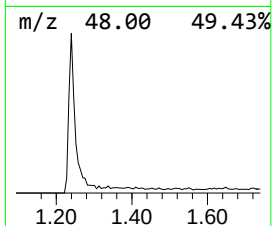
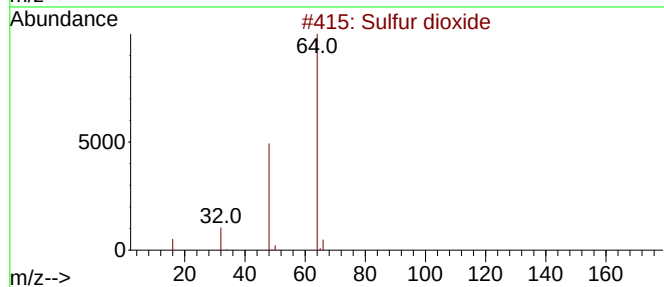
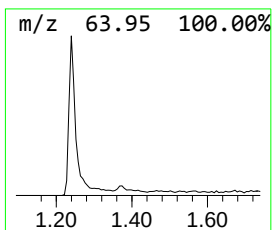
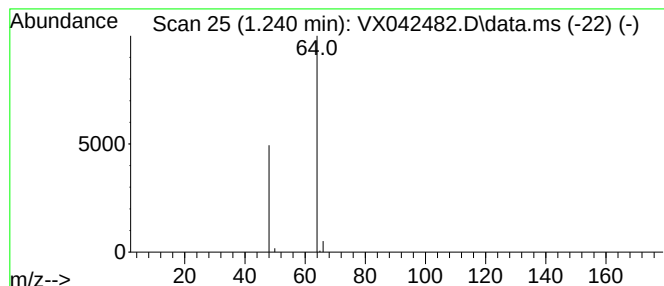
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	3.52 ug/L	28941	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Sulfur dioxide	64	O2S	007446-09-5	4



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.5	ug/L	28941	1	6.763	411130	50.0