

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041923\
 Data File : VX035175.D
 Acq On : 19 Apr 2023 17:24
 Operator : JC/MD
 Sample : 02333-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMG8

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035175.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	43	rBV	167195	372364	4.61%	1.320%
2	1.368	43	46	58	rVB	163561	185383	2.29%	0.657%
3	1.672	92	96	107	rVB	116468	150701	1.87%	0.534%
4	2.306	194	200	211	rBV	309410	487106	6.03%	1.726%
5	2.508	231	233	242	rVB3	675	1117	0.01%	0.004%
6	2.581	244	245	247	rBV	412	267	0.00%	0.001%
7	2.788	275	279	282	rBV3	913	1294	0.02%	0.005%
8	2.861	288	291	292	rBV	488	465	0.01%	0.002%
9	2.928	299	302	303	rBV3	680	736	0.01%	0.003%
10	3.020	314	317	319	rBV	262	311	0.00%	0.001%
11	3.160	336	340	341	rBV2	222	292	0.00%	0.001%
12	3.264	356	357	361	rVV	299	268	0.00%	0.001%
13	3.434	383	385	387	rVB2	327	225	0.00%	0.001%
14	3.465	387	390	392	rBV	256	310	0.00%	0.001%
15	3.629	414	417	419	rBV2	248	224	0.00%	0.001%
16	3.721	431	432	436	rVV	207	243	0.00%	0.001%
17	3.831	448	450	453	rVV2	200	228	0.00%	0.001%
18	3.916	463	464	468	rBV	270	228	0.00%	0.001%
19	4.001	477	478	483	rVV	269	368	0.00%	0.001%
20	4.099	489	494	496	rBV2	241	422	0.01%	0.001%
21	4.306	521	528	534	rBV5	1421	3498	0.04%	0.012%
22	4.385	540	541	543	rVB	382	225	0.00%	0.001%
23	4.465	545	554	576	rBV	79288	258539	3.20%	0.916%
24	4.702	591	593	594	rVB	570	342	0.00%	0.001%
25	4.812	609	611	614	rVB3	265	278	0.00%	0.001%
26	4.873	619	621	622	rBV2	277	229	0.00%	0.001%
27	4.940	630	632	635	rVB2	320	288	0.00%	0.001%
28	5.056	638	651	669	rBV2	175182	529386	6.55%	1.876%
29	5.391	701	706	708	rBV4	742	1207	0.01%	0.004%
30	5.556	726	733	745	rVB3	2107	6501	0.08%	0.023%
31	5.678	745	753	760	rBV3	3114	9459	0.12%	0.034%
32	5.970	789	801	805	rBV2	471025	1320374	16.34%	4.679%
33	6.037	806	812	831	rVB	1653810	4302303	53.26%	15.247%
34	6.275	849	851	852	rBV	399	304	0.00%	0.001%
35	6.373	866	867	870	rBV2	404	283	0.00%	0.001%
36	6.452	879	880	883	rBV2	402	398	0.00%	0.001%

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 Title : VOC Analysis

37	6.531	891	893	894	rBV	329	312	0.00%	0.001%
38	6.763	921	931	945	rBV	482339	1162253	14.39%	4.119%
39	6.988	967	968	972	rBV2	256	299	0.00%	0.001%
40	7.104	985	987	989	rBV2	640	706	0.01%	0.003%
41	7.305	1011	1020	1037	rBV	280812	618219	7.65%	2.191%
42	7.488	1046	1050	1058	rVB6	866	2135	0.03%	0.008%
43	7.543	1058	1059	1061	rBV	445	248	0.00%	0.001%
44	7.952	1121	1126	1128	rVV4	701	1024	0.01%	0.004%
45	8.019	1134	1137	1138	rBV	294	279	0.00%	0.001%
46	8.324	1181	1187	1201	rBV	141209	232464	2.88%	0.824%
47	8.647	1233	1240	1261	rBV	722692	1147591	14.21%	4.067%
48	8.854	1273	1274	1279	rBV3	423	394	0.00%	0.001%
49	8.952	1284	1290	1302	rBV	95356	143277	1.77%	0.508%
50	9.208	1329	1332	1334	rBV2	318	382	0.00%	0.001%
51	9.275	1337	1343	1346	rBV3	2642	3094	0.04%	0.011%
52	9.384	1356	1361	1380	rBV	378266	562381	6.96%	1.993%
53	9.683	1408	1410	1412	rBV2	351	316	0.00%	0.001%
54	9.939	1448	1452	1458	rBV2	508	667	0.01%	0.002%
55	10.079	1465	1475	1492	rBV2	5043937	8078552	100.00%	28.630%
56	10.457	1535	1537	1538	rVB2	519	297	0.00%	0.001%
57	10.579	1556	1557	1562	rVV3	219	244	0.00%	0.001%
58	10.640	1566	1567	1570	rBV	285	340	0.00%	0.001%
59	10.695	1575	1576	1580	rVB2	442	483	0.01%	0.002%
60	10.811	1592	1595	1596	rVB	357	238	0.00%	0.001%
61	10.957	1617	1619	1621	rBV2	490	315	0.00%	0.001%
62	11.012	1625	1628	1629	rBV2	322	256	0.00%	0.001%
63	11.073	1634	1638	1641	rBV2	243	365	0.00%	0.001%
64	11.189	1652	1657	1673	rVV	445792	593722	7.35%	2.104%
65	11.317	1676	1678	1683	rVB2	927	825	0.01%	0.003%
66	11.372	1683	1687	1690	rVB3	882	1243	0.02%	0.004%
67	11.427	1690	1696	1698	rBV3	449	790	0.01%	0.003%
68	11.457	1698	1701	1703	rBV2	449	483	0.01%	0.002%
69	11.640	1726	1731	1733	rBV2	187	295	0.00%	0.001%
70	11.707	1740	1742	1746	rVB	346	436	0.01%	0.002%
71	11.744	1746	1748	1749	rBV2	323	291	0.00%	0.001%
72	11.756	1749	1750	1752	rVV	497	339	0.00%	0.001%
73	11.805	1756	1758	1761	rVB2	247	303	0.00%	0.001%
74	11.969	1780	1785	1789	rBV	150123	187127	2.32%	0.663%
75	12.042	1789	1797	1809	rVB2	2350118	4174461	51.67%	14.794%
76	12.219	1823	1826	1834	rVB2	3055	4702	0.06%	0.017%

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Peak Location: TOP

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77	12.335	1837	1845	1864	rVB2	2112418	3346023	41.42%	11.858%
78	12.548	1878	1880	1884	rBV4	383	665	0.01%	0.002%
79	12.670	1899	1900	1905	rBV2	338	421	0.01%	0.001%
80	12.719	1905	1908	1910	rBV2	295	363	0.00%	0.001%
81	12.762	1913	1915	1920	rVB4	475	510	0.01%	0.002%
82	12.841	1926	1928	1929	rBV	267	229	0.00%	0.001%
83	13.061	1958	1964	1967	rBV3	361	705	0.01%	0.002%
84	13.115	1971	1973	1976	rVB3	526	636	0.01%	0.002%
85	13.195	1984	1986	1989	rVB2	324	310	0.00%	0.001%
86	13.378	2013	2016	2019	rVB2	259	351	0.00%	0.001%
87	13.585	2045	2050	2059	rBV	200524	259463	3.21%	0.920%
88	13.737	2073	2075	2079	rBV	330	396	0.00%	0.001%
89	13.774	2079	2081	2085	rBV2	463	608	0.01%	0.002%
90	13.963	2107	2112	2118	rVV	20896	27274	0.34%	0.097%
91	14.341	2172	2174	2178	rBV	374	641	0.01%	0.002%
92	14.420	2184	2187	2188	rBV2	442	452	0.01%	0.002%
93	14.572	2210	2212	2214	rVB2	519	328	0.00%	0.001%
94	14.786	2242	2247	2251	rBV4	4531	6170	0.08%	0.022%
95	14.853	2255	2258	2259	rBV2	552	601	0.01%	0.002%
96	15.249	2319	2323	2328	rBV3	8032	10555	0.13%	0.037%
97	15.408	2347	2349	2350	rBV	502	276	0.00%	0.001%
98	16.036	2451	2452	2454	rBV2	658	431	0.01%	0.002%
99	16.566	2537	2539	2541	rBV2	650	595	0.01%	0.002%
100	16.731	2564	2566	2568	rBV2	829	813	0.01%	0.003%

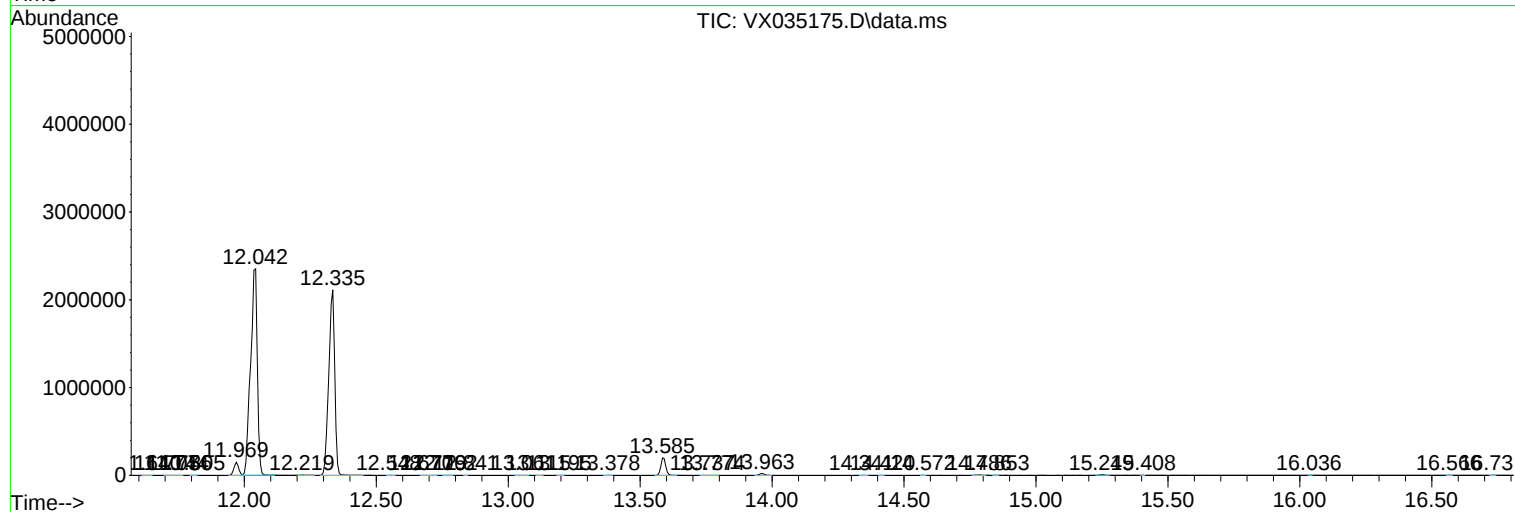
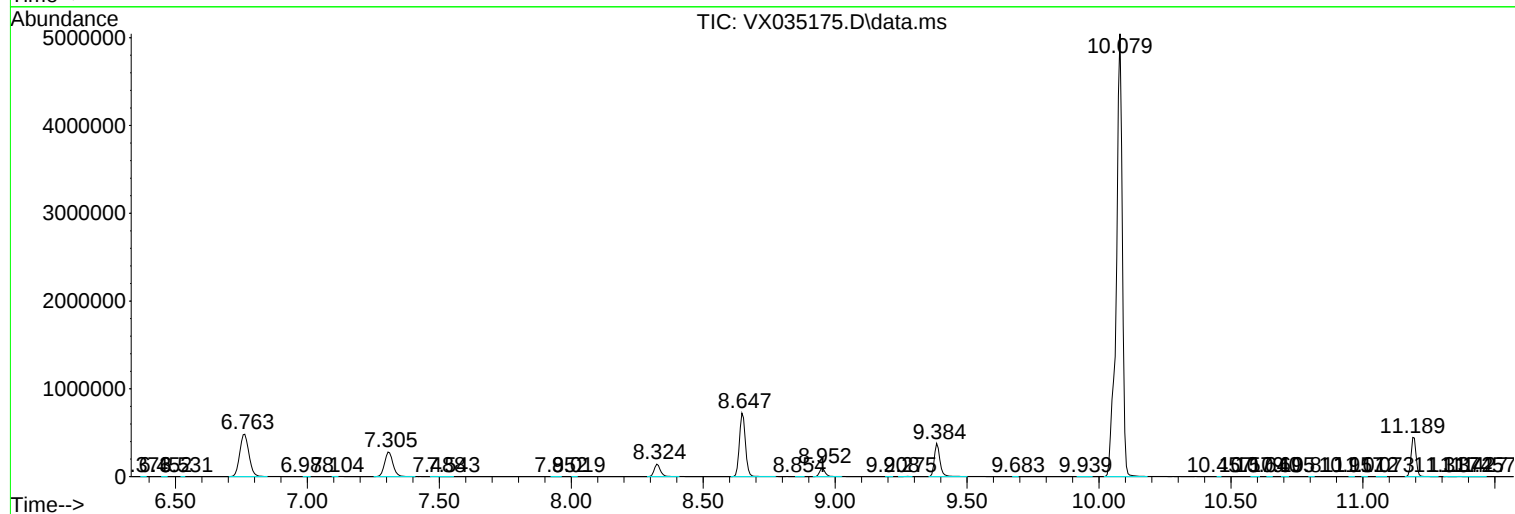
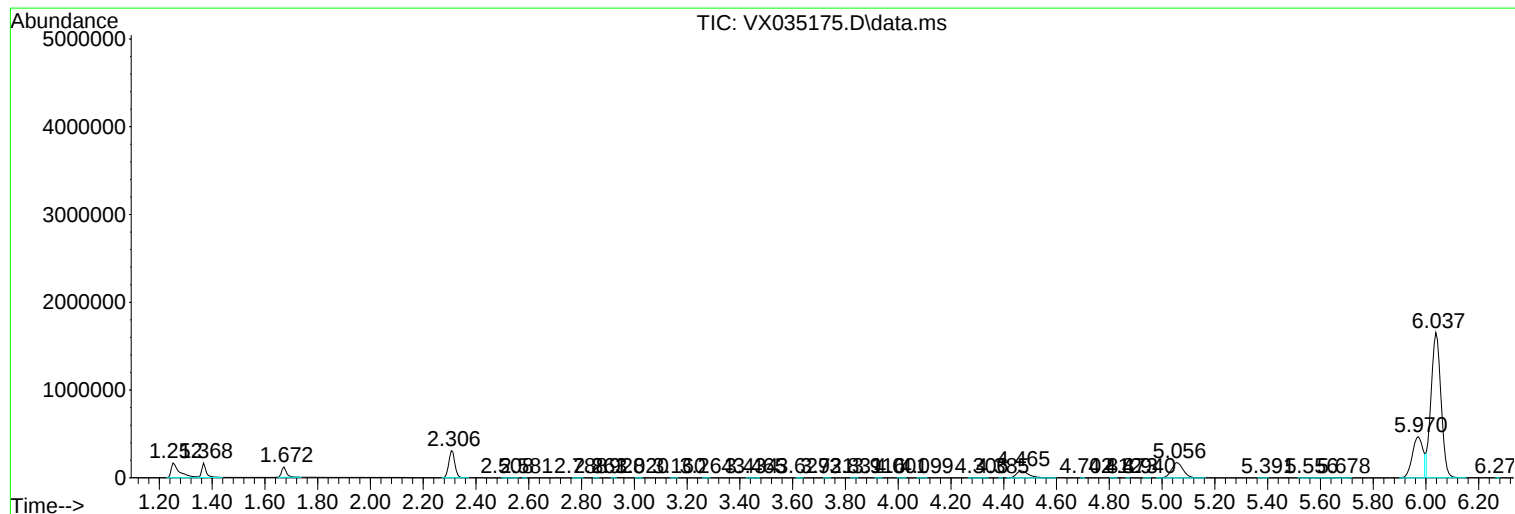
Sum of corrected areas: 28217130

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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VOX041923\
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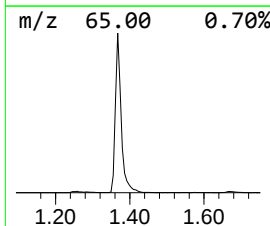
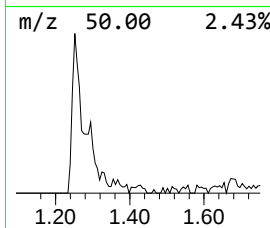
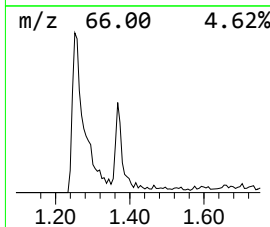
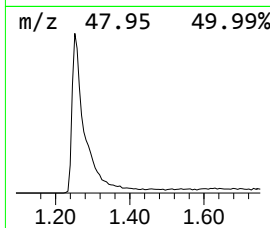
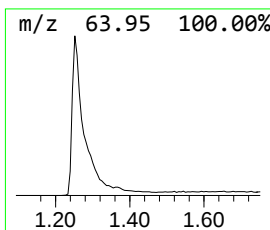
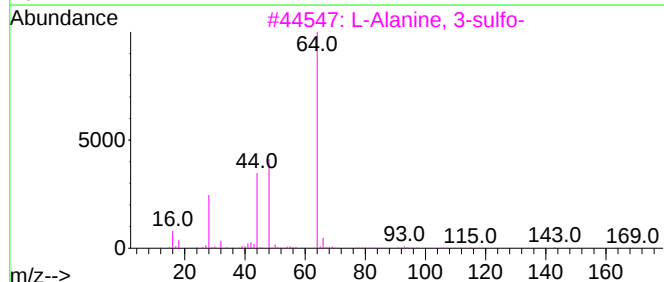
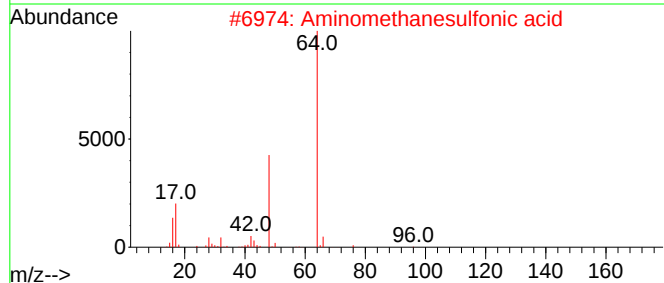
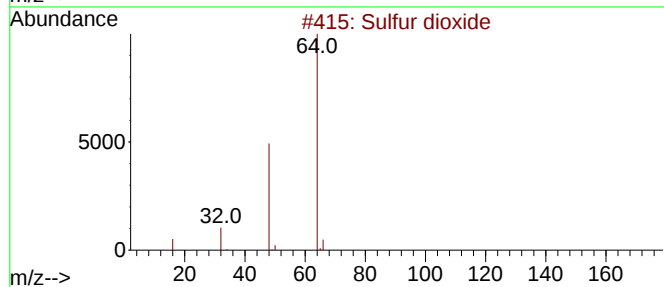
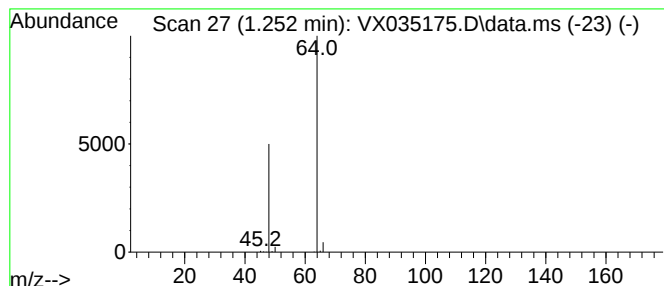
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	16.02 ug/L	372364	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	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.252	16.0	ug/L	372364	1	6.763	1162250	50.0