

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081022\
 Data File : VX030551.D
 Acq On : 10 Aug 2022 14:47
 Operator : JC/MD
 Sample : N4076-06DL 10X
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBUU6DL

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\SFAMXML080422WMA.M

Title : VOC Analysis

Signal : TIC: VX030551.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	42	rBV	132225	253045	19.16%	2.440%
2	1.368	42	46	57	rVB	164684	170820	12.93%	1.647%
3	1.666	91	95	104	rVB	128742	155242	11.75%	1.497%
4	2.307	194	200	209	rVB	283046	423254	32.04%	4.082%
5	2.788	276	279	285	rBB6	1411	2565	0.19%	0.025%
6	2.880	293	294	298	rBV2	721	1080	0.08%	0.010%
7	2.947	299	305	315	rVB2	8384	19075	1.44%	0.184%
8	3.093	322	329	338	rVB	45712	87005	6.59%	0.839%
9	3.312	363	365	367	rBV2	532	711	0.05%	0.007%
10	3.404	379	380	383	rBV3	482	437	0.03%	0.004%
11	3.447	385	387	388	rBV2	544	342	0.03%	0.003%
12	3.684	423	426	428	rBV3	455	561	0.04%	0.005%
13	3.757	436	438	439	rBV	577	382	0.03%	0.004%
14	3.849	451	453	457	rVB3	802	852	0.06%	0.008%
15	4.184	504	508	509	rBV2	983	1236	0.09%	0.012%
16	4.318	528	530	531	rBV2	555	346	0.03%	0.003%
17	4.489	546	558	571	rBV2	218370	707734	53.58%	6.825%
18	4.721	594	596	598	rBV3	762	479	0.04%	0.005%
19	4.958	633	635	637	rVB	641	430	0.03%	0.004%
20	5.062	641	652	668	rVV	177895	550046	41.64%	5.305%
21	5.696	754	756	759	rBV3	683	802	0.06%	0.008%
22	5.879	784	786	790	rBV3	398	490	0.04%	0.005%
23	5.977	790	802	815	rBV2	462291	1320951	100.00%	12.739%
24	6.208	838	840	841	rBV	648	390	0.03%	0.004%
25	6.464	880	882	883	rBV	434	318	0.02%	0.003%
26	6.769	922	932	946	rBV	288460	690630	52.28%	6.660%
27	7.117	983	989	997	rVB5	7713	18241	1.38%	0.176%
28	7.202	1001	1003	1007	rVB4	532	462	0.03%	0.004%
29	7.312	1011	1021	1035	rBV	270437	609477	46.14%	5.878%
30	7.550	1058	1060	1063	rVB2	571	450	0.03%	0.004%
31	7.836	1104	1107	1108	rBV2	546	598	0.05%	0.006%
32	7.940	1122	1124	1127	rVV4	696	691	0.05%	0.007%
33	8.141	1153	1157	1158	rBV2	551	702	0.05%	0.007%
34	8.244	1172	1174	1176	rBV2	286	328	0.02%	0.003%
35	8.330	1181	1188	1201	rBV	187315	309723	23.45%	2.987%
36	8.653	1234	1241	1252	rBV	667031	1021759	77.35%	9.854%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

37	8.952	1285	1290	1303	rBV	137133	206506	15.63%	1.992%
38	9.214	1332	1333	1334	rBV	673	426	0.03%	0.004%
39	9.281	1340	1344	1346	rVB	1100	1244	0.09%	0.012%
40	9.391	1356	1362	1373	rBV	531163	751979	56.93%	7.252%
41	9.726	1415	1417	1418	rVB2	584	356	0.03%	0.003%
42	9.781	1425	1426	1428	rBV2	459	359	0.03%	0.003%
43	9.939	1449	1452	1454	rBV2	384	410	0.03%	0.004%
44	9.988	1458	1460	1465	rBV2	426	784	0.06%	0.008%
45	10.055	1465	1471	1481	rBV	612343	815513	61.74%	7.865%
46	10.226	1497	1499	1500	rBV2	487	434	0.03%	0.004%
47	10.378	1521	1524	1532	rVB4	1548	2478	0.19%	0.024%
48	10.482	1537	1541	1542	rBV3	402	592	0.04%	0.006%
49	10.549	1550	1552	1555	rBV3	457	455	0.03%	0.004%
50	10.647	1566	1568	1569	rBV2	621	427	0.03%	0.004%
51	10.665	1569	1571	1573	rVB	620	423	0.03%	0.004%
52	10.720	1578	1580	1583	rVV2	529	513	0.04%	0.005%
53	10.848	1600	1601	1604	rVB	533	383	0.03%	0.004%
54	10.878	1604	1606	1610	rBV2	483	720	0.05%	0.007%
55	10.909	1610	1611	1615	rVB2	438	473	0.04%	0.005%
56	10.964	1615	1620	1623	rBV2	643	900	0.07%	0.009%
57	10.988	1623	1624	1627	rVB3	522	333	0.03%	0.003%
58	11.018	1627	1629	1631	rBV2	517	529	0.04%	0.005%
59	11.195	1652	1658	1669	rVB	481909	614738	46.54%	5.928%
60	11.439	1697	1698	1700	rBV2	406	341	0.03%	0.003%
61	11.628	1728	1729	1731	rBV	769	445	0.03%	0.004%
62	11.756	1748	1750	1752	rBV	434	398	0.03%	0.004%
63	11.890	1769	1772	1776	rVV3	891	1151	0.09%	0.011%
64	12.024	1789	1794	1802	rBV	604616	733280	55.51%	7.072%
65	12.104	1806	1807	1810	rBV3	684	497	0.04%	0.005%
66	12.323	1837	1843	1851	rBV	692430	860503	65.14%	8.299%
67	12.713	1905	1907	1908	rBV2	607	475	0.04%	0.005%
68	12.866	1931	1932	1934	rBV2	537	429	0.03%	0.004%
69	12.890	1934	1936	1937	rVV2	605	461	0.03%	0.004%
70	12.908	1937	1939	1943	rVV3	682	841	0.06%	0.008%
71	12.939	1943	1944	1945	rVV	665	367	0.03%	0.004%
72	13.116	1971	1973	1976	rBV2	551	512	0.04%	0.005%
73	13.140	1976	1977	1980	rVB3	470	389	0.03%	0.004%
74	13.268	1997	1998	2003	rBV3	637	749	0.06%	0.007%
75	13.347	2008	2011	2013	rBV2	423	488	0.04%	0.005%
76	13.402	2018	2020	2023	rVB	571	460	0.03%	0.004%

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Smoothing : OFF

Filtering: 5

Sampling : 1

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Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

77	13.506	2035	2037	2040	rVB	432	463	0.04%	0.004%
78	13.573	2045	2048	2049	rBV2	709	583	0.04%	0.006%
79	13.670	2062	2064	2066	rVV3	648	486	0.04%	0.005%
80	13.707	2068	2070	2073	rVV2	624	610	0.05%	0.006%
81	13.731	2073	2074	2077	rVV	517	382	0.03%	0.004%
82	13.774	2080	2081	2084	rBV2	490	469	0.04%	0.005%
83	13.847	2091	2093	2096	rBV2	512	439	0.03%	0.004%
84	13.933	2104	2107	2109	rVB2	715	774	0.06%	0.007%
85	13.963	2109	2112	2114	rBV3	787	1000	0.08%	0.010%
86	14.085	2130	2132	2133	rBV2	655	460	0.03%	0.004%
87	14.195	2144	2150	2151	rBV5	1980	2908	0.22%	0.028%
88	14.487	2196	2198	2200	rBV2	779	661	0.05%	0.006%
89	14.603	2214	2217	2218	rBV2	359	305	0.02%	0.003%
90	14.621	2218	2220	2221	rBV2	492	308	0.02%	0.003%
91	14.640	2221	2223	2226	rVB3	624	606	0.05%	0.006%
92	14.768	2243	2244	2246	rVB	614	403	0.03%	0.004%
93	14.810	2249	2251	2252	rBV2	461	300	0.02%	0.003%
94	15.024	2284	2286	2287	rBV2	603	500	0.04%	0.005%
95	15.109	2295	2300	2302	rBV4	851	1151	0.09%	0.011%
96	15.286	2327	2329	2331	rBV2	506	535	0.04%	0.005%
97	15.566	2373	2375	2377	rBV	518	493	0.04%	0.005%
98	15.633	2385	2386	2388	rBV	700	405	0.03%	0.004%
99	15.682	2392	2394	2395	rBV2	610	303	0.02%	0.003%
100	16.560	2536	2538	2541	rBV3	604	360	0.03%	0.003%

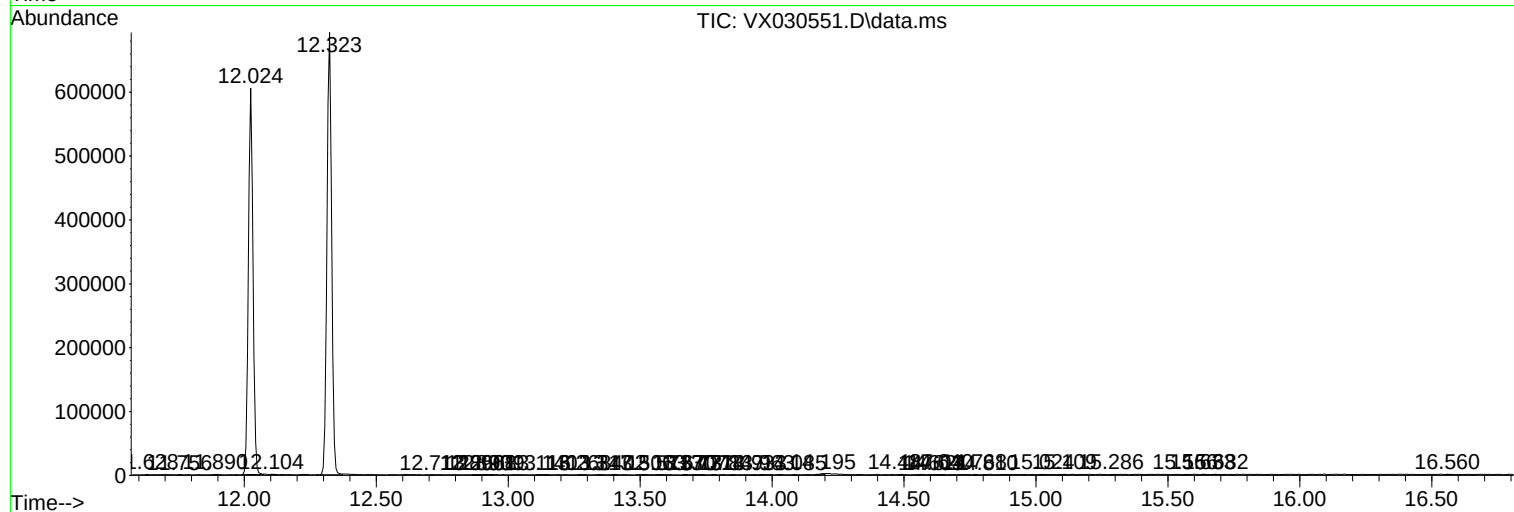
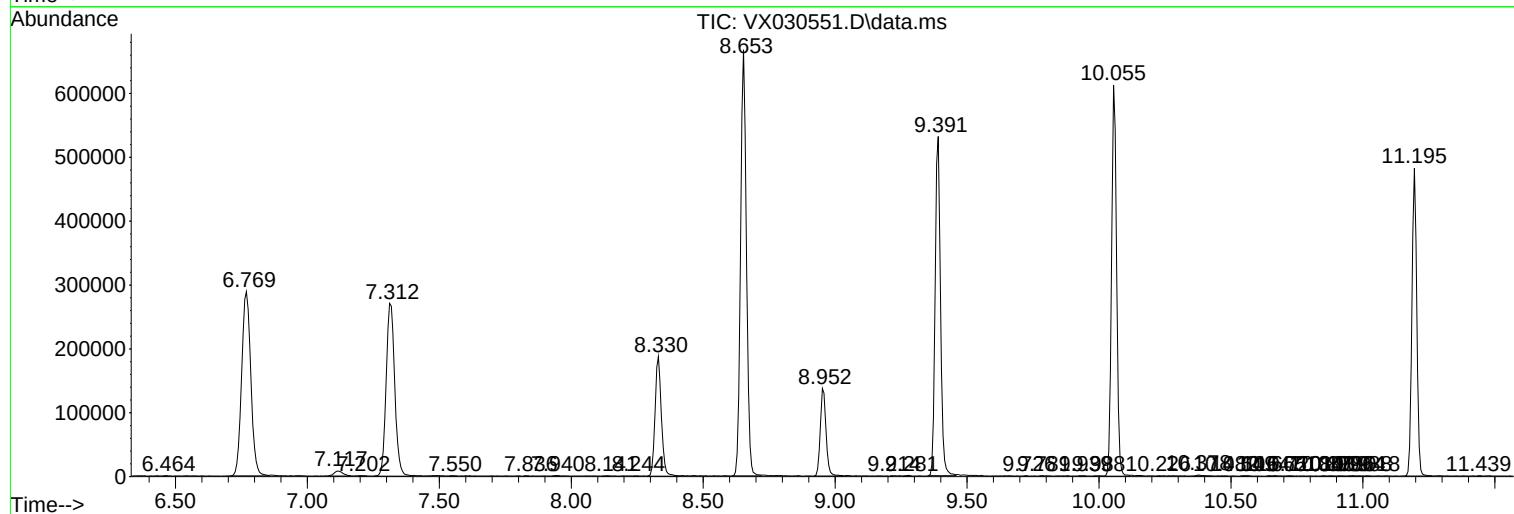
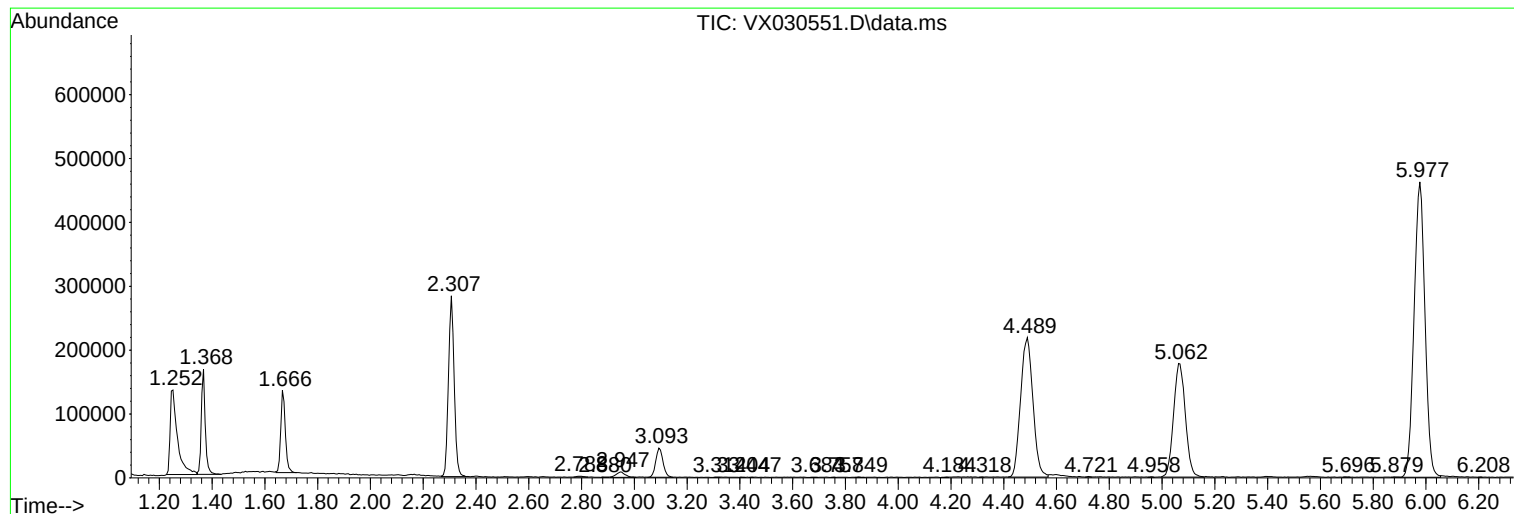
Sum of corrected areas: 10369319

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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



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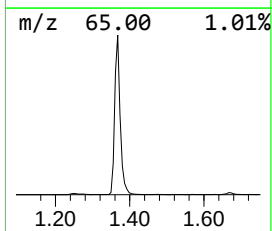
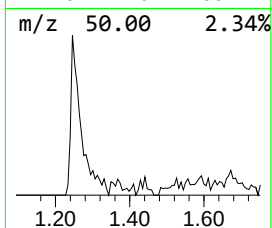
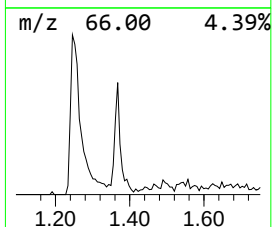
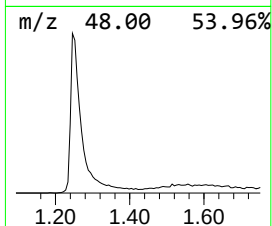
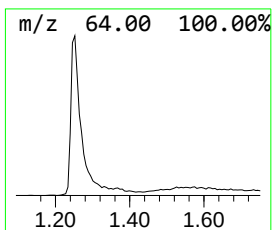
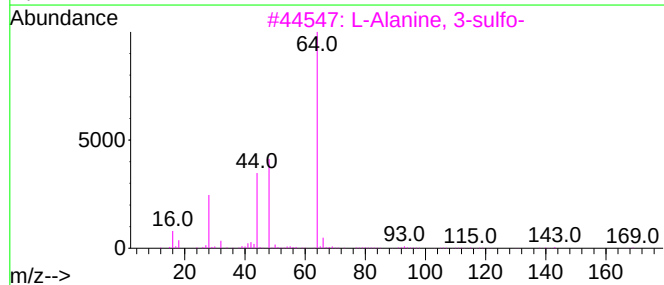
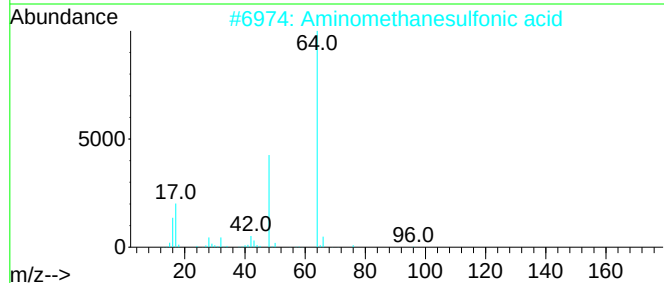
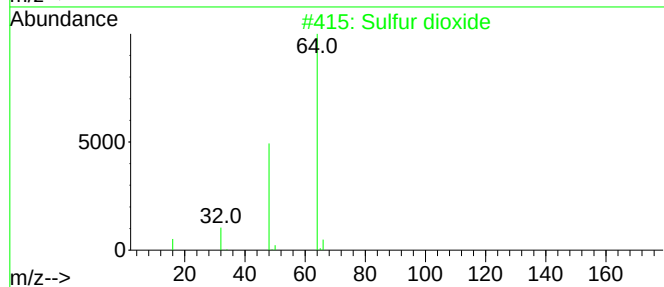
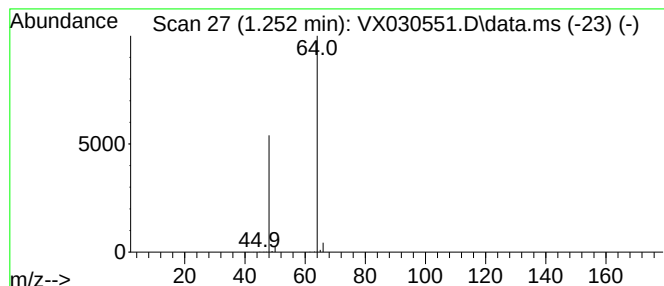
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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.
1.252	18.32 ug/L	253045	1,4-Difluorobenzene	6.769

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			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	18.3	ug/L	253045	1	6.769	690630	50.0