

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081022\
 Data File : VX030559.D
 Acq On : 10 Aug 2022 17:55
 Operator : JC/MD
 Sample : VIBLK667
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VIBLK667

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: VX030559.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	92510	185179	14.58%	1.928%
2	1.368	42	46	55	rVB	147209	155439	12.24%	1.618%
3	1.666	91	95	102	rVB	118145	144529	11.38%	1.505%
4	2.306	194	200	212	rVB	239412	375359	29.56%	3.908%
5	2.660	257	258	265	rBV4	550	1025	0.08%	0.011%
6	2.788	275	279	285	rVB7	1768	3448	0.27%	0.036%
7	2.947	298	305	313	rVV	6352	14170	1.12%	0.148%
8	3.026	316	318	323	rVB2	334	365	0.03%	0.004%
9	3.136	334	336	338	rVV2	527	463	0.04%	0.005%
10	3.215	347	349	352	rBV3	445	468	0.04%	0.005%
11	3.434	382	385	390	rBV3	638	931	0.07%	0.010%
12	3.520	395	399	400	rVB3	381	384	0.03%	0.004%
13	3.703	426	429	431	rVB3	315	342	0.03%	0.004%
14	3.733	431	434	435	rBV3	492	538	0.04%	0.006%
15	3.782	440	442	443	rVV2	568	359	0.03%	0.004%
16	3.806	445	446	451	rVB3	677	453	0.04%	0.005%
17	3.843	451	452	455	rVB2	396	365	0.03%	0.004%
18	3.879	455	458	460	rBV	620	634	0.05%	0.007%
19	4.099	492	494	496	rVB	402	343	0.03%	0.004%
20	4.135	498	500	504	rVB2	584	579	0.05%	0.006%
21	4.196	508	510	511	rBV2	520	374	0.03%	0.004%
22	4.477	547	556	573	rBV2	113569	339252	26.71%	3.532%
23	5.068	641	653	670	rVB	170399	514793	40.54%	5.359%
24	5.403	706	708	710	rVB	994	526	0.04%	0.005%
25	5.464	717	718	722	rBV3	409	469	0.04%	0.005%
26	5.812	773	775	777	rBV2	531	636	0.05%	0.007%
27	5.976	790	802	820	rBV2	439431	1269909	100.00%	13.220%
28	6.354	862	864	865	rVB	803	446	0.04%	0.005%
29	6.690	916	919	922	rVB4	650	735	0.06%	0.008%
30	6.769	922	932	951	rBV2	301633	717395	56.49%	7.468%
31	7.117	982	989	997	rVV6	8806	21319	1.68%	0.222%
32	7.245	1006	1010	1011	rBV	427	447	0.04%	0.005%
33	7.312	1013	1021	1034	rVV	264173	591576	46.58%	6.159%
34	7.476	1046	1048	1059	rVB7	1263	3160	0.25%	0.033%
35	7.696	1083	1084	1087	rVB3	480	407	0.03%	0.004%
36	8.330	1182	1188	1198	rVV	175834	286759	22.58%	2.985%

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Integrator: RTE

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 Title : VOC Analysis

37	8.555	1223	1225	1227	rBV2	441	417	0.03%	0.004%
38	8.653	1231	1241	1251	rBV	623836	975084	76.78%	10.151%
39	8.891	1278	1280	1283	rVB2	580	444	0.03%	0.005%
40	8.952	1283	1290	1303	rBV	127471	196900	15.51%	2.050%
41	9.323	1348	1351	1353	rBV3	680	909	0.07%	0.009%
42	9.391	1356	1362	1377	rBV	525022	738357	58.14%	7.687%
43	9.708	1409	1414	1417	rVB4	2720	3422	0.27%	0.036%
44	9.915	1444	1448	1452	rVB3	608	847	0.07%	0.009%
45	9.945	1452	1453	1456	rBV3	646	498	0.04%	0.005%
46	9.970	1456	1457	1462	rVB2	514	600	0.05%	0.006%
47	10.055	1466	1471	1479	rBV	584185	806113	63.48%	8.392%
48	10.177	1490	1491	1493	rBV2	604	547	0.04%	0.006%
49	10.238	1500	1501	1505	rVB2	623	611	0.05%	0.006%
50	10.342	1517	1518	1521	rBV2	384	428	0.03%	0.004%
51	10.488	1540	1542	1548	rBV4	503	964	0.08%	0.010%
52	10.579	1554	1557	1562	rBV2	591	1263	0.10%	0.013%
53	10.646	1566	1568	1570	rVB3	599	508	0.04%	0.005%
54	10.744	1583	1584	1587	rBV3	366	392	0.03%	0.004%
55	10.787	1589	1591	1594	rBV2	670	532	0.04%	0.006%
56	10.890	1606	1608	1612	rVV3	305	375	0.03%	0.004%
57	11.195	1653	1658	1667	rVB	488521	597334	47.04%	6.219%
58	11.366	1685	1686	1688	rBV2	489	356	0.03%	0.004%
59	11.439	1697	1698	1701	rBV2	472	455	0.04%	0.005%
60	11.549	1714	1716	1719	rVB2	472	366	0.03%	0.004%
61	11.634	1728	1730	1731	rBV2	455	397	0.03%	0.004%
62	11.671	1734	1736	1737	rBV2	665	440	0.03%	0.005%
63	11.786	1752	1755	1756	rVB2	440	360	0.03%	0.004%
64	11.847	1763	1765	1767	rBV	355	439	0.03%	0.005%
65	11.884	1770	1771	1774	rVB2	647	367	0.03%	0.004%
66	11.969	1783	1785	1788	rVB2	529	511	0.04%	0.005%
67	12.024	1789	1794	1801	rVV	644122	749929	59.05%	7.807%
68	12.219	1825	1826	1828	rBV2	727	392	0.03%	0.004%
69	12.268	1833	1834	1837	rBV	420	484	0.04%	0.005%
70	12.323	1837	1843	1852	rBV	691316	874652	68.88%	9.106%
71	12.481	1866	1869	1870	rBV2	403	426	0.03%	0.004%
72	12.555	1878	1881	1882	rBV3	530	517	0.04%	0.005%
73	12.579	1882	1885	1887	rBV3	440	460	0.04%	0.005%
74	12.829	1924	1926	1928	rBV3	441	347	0.03%	0.004%
75	12.853	1928	1930	1933	rVB2	669	532	0.04%	0.006%
76	12.951	1945	1946	1947	rBV	751	385	0.03%	0.004%

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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

77	13.006	1953	1955	1957	rBV	463	483	0.04%	0.005%
78	13.103	1969	1971	1974	rBV2	652	621	0.05%	0.006%
79	13.140	1974	1977	1980	rBV2	542	679	0.05%	0.007%
80	13.237	1991	1993	1994	rVB2	727	423	0.03%	0.004%
81	13.457	2027	2029	2030	rBV	428	354	0.03%	0.004%
82	13.597	2050	2052	2054	rBV2	556	491	0.04%	0.005%
83	13.646	2058	2060	2063	rBV3	473	548	0.04%	0.006%
84	13.682	2065	2066	2069	rBV3	589	491	0.04%	0.005%
85	13.713	2069	2071	2073	rBV	663	503	0.04%	0.005%
86	14.012	2119	2120	2121	rBV	610	361	0.03%	0.004%
87	14.195	2147	2150	2151	rBV2	884	1050	0.08%	0.011%
88	14.323	2170	2171	2175	rVB2	753	545	0.04%	0.006%
89	14.359	2175	2177	2181	rBV4	551	750	0.06%	0.008%
90	14.438	2189	2190	2193	rVB2	612	523	0.04%	0.005%
91	14.512	2201	2202	2203	rBV	565	341	0.03%	0.004%
92	14.676	2226	2229	2232	rBV3	419	666	0.05%	0.007%
93	14.902	2264	2266	2268	rVB	842	583	0.05%	0.006%
94	15.036	2287	2288	2291	rBV2	671	588	0.05%	0.006%
95	15.085	2293	2296	2298	rBV4	728	889	0.07%	0.009%
96	15.341	2336	2338	2340	rBV2	569	439	0.03%	0.005%
97	15.767	2406	2408	2409	rBV2	495	520	0.04%	0.005%
98	16.054	2451	2455	2457	rBV4	665	827	0.07%	0.009%
99	16.493	2524	2527	2528	rBV3	727	661	0.05%	0.007%
100	16.590	2541	2543	2544	rBV2	847	468	0.04%	0.005%

Sum of corrected areas: 9605740

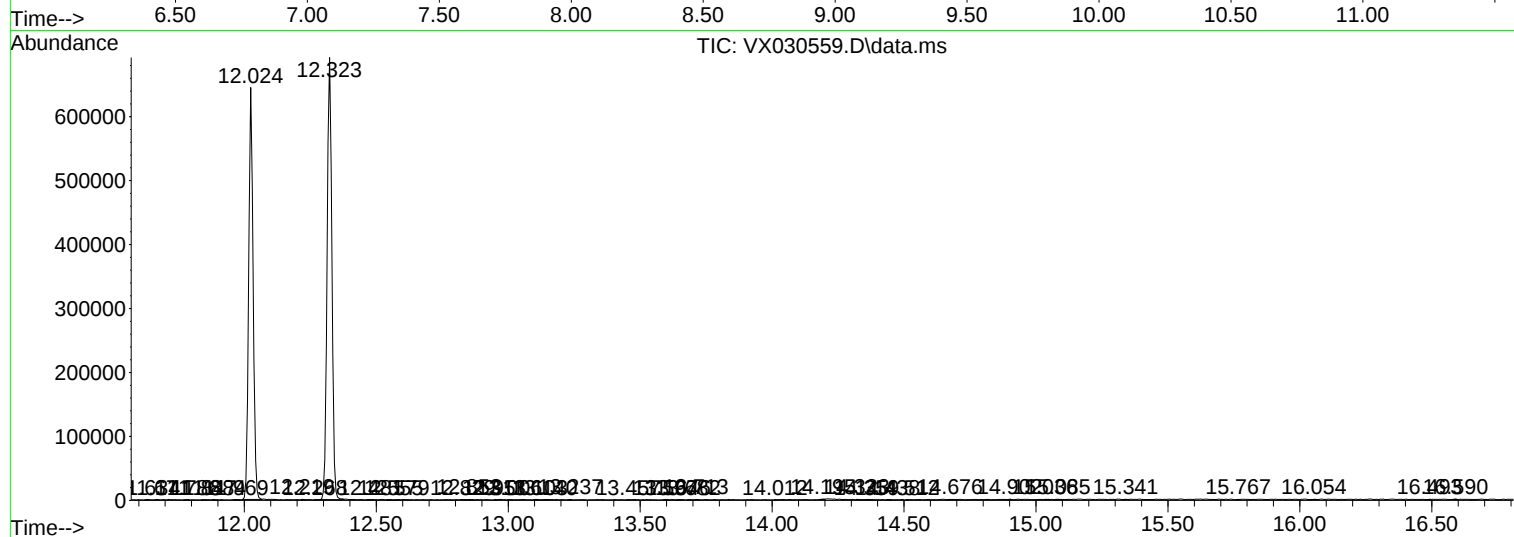
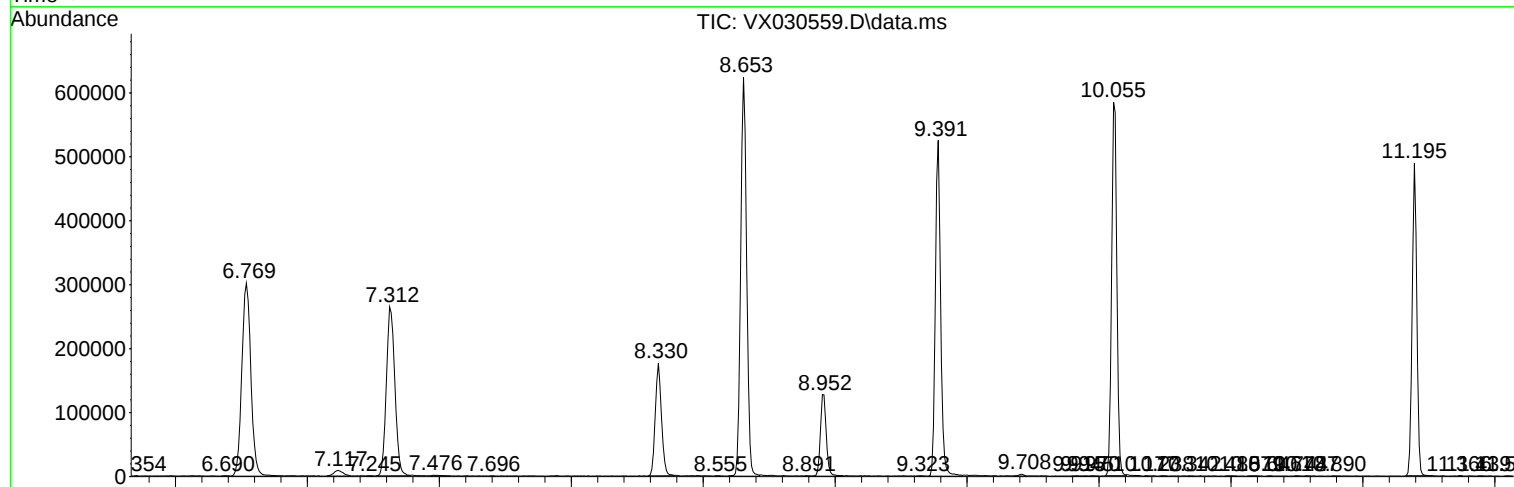
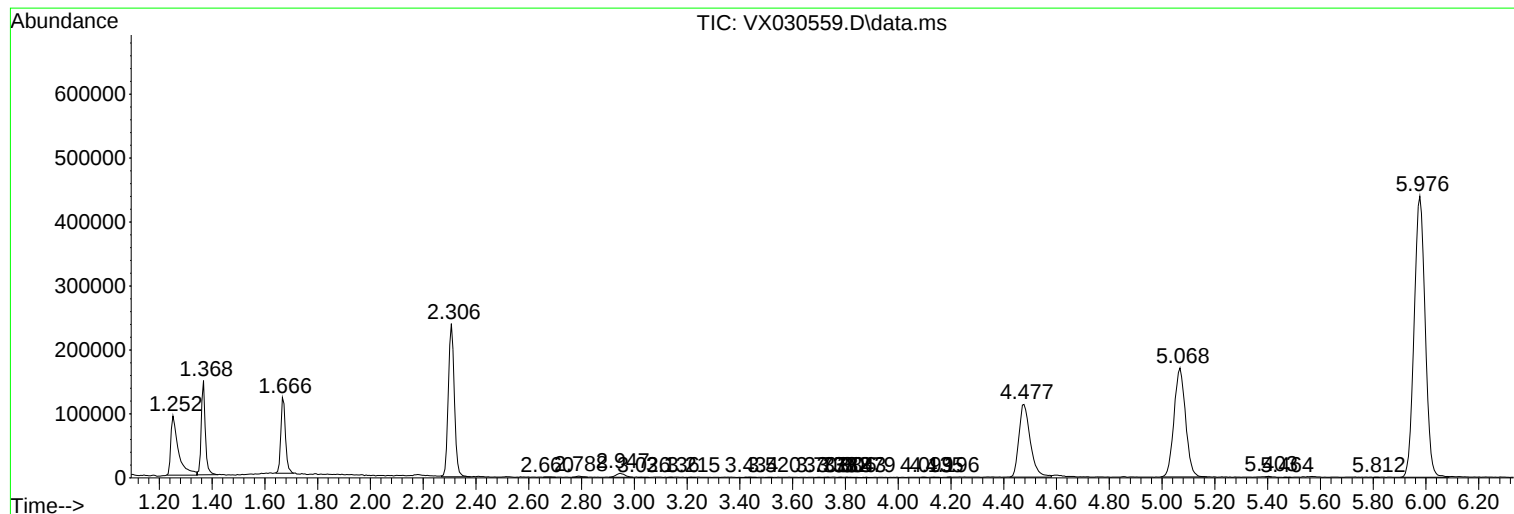
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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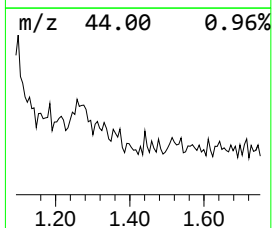
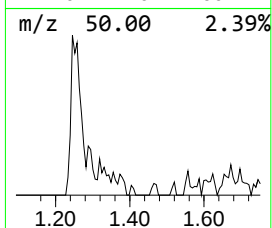
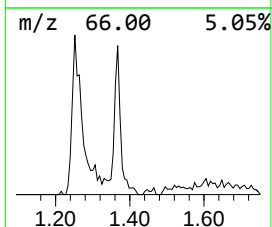
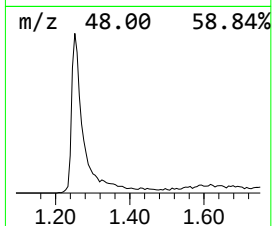
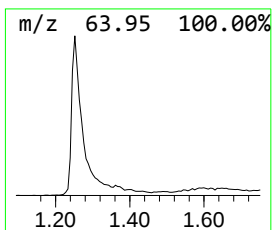
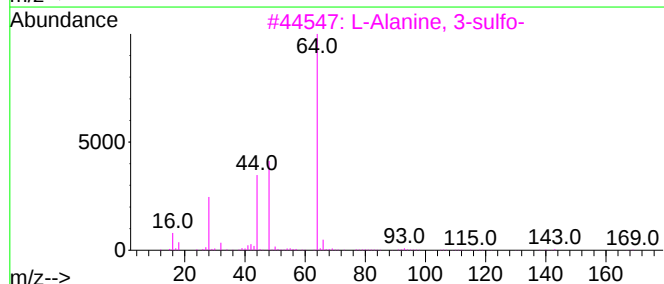
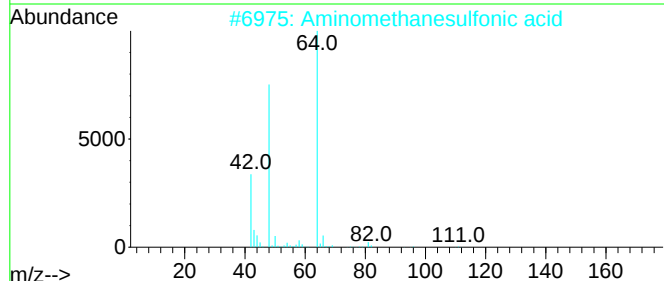
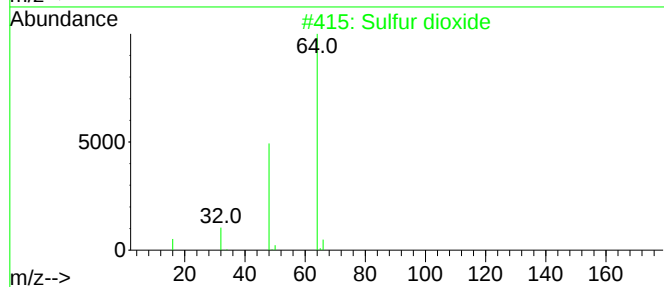
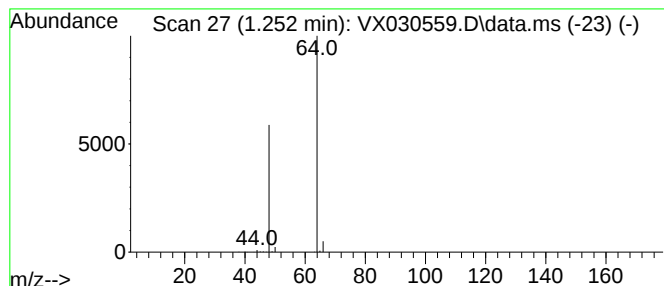
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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	12.91 ug/L	185179	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	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	12.9	ug/L	185179	1	6.769	717395	50.0