

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080922\
 Data File : VX030533.D
 Acq On : 09 Aug 2022 17:34
 Operator : JC/MD
 Sample : N4114-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 F5D75

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: VX030533.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	40	rBV	37423	85877	8.95%	1.017%
2	1.368	43	46	57	rVB2	202995	244628	25.49%	2.897%
3	1.666	92	95	104	rVB	80522	102362	10.67%	1.212%
4	2.307	194	200	211	rVB	173172	262795	27.38%	3.113%
5	2.642	253	255	257	rVB2	667	585	0.06%	0.007%
6	2.678	257	261	262	rBV3	780	1044	0.11%	0.012%
7	2.855	287	290	293	rBV3	437	560	0.06%	0.007%
8	2.941	300	304	305	rBV2	596	561	0.06%	0.007%
9	3.020	315	317	323	rVB3	864	1059	0.11%	0.013%
10	3.099	323	330	337	rBV2	24585	46822	4.88%	0.555%
11	3.166	337	341	344	rVB2	486	536	0.06%	0.006%
12	3.270	355	358	360	rBV2	781	830	0.09%	0.010%
13	3.441	384	386	389	rVB3	449	460	0.05%	0.005%
14	3.569	404	407	408	rBV3	416	396	0.04%	0.005%
15	3.648	418	420	421	rBV3	464	415	0.04%	0.005%
16	3.739	431	435	436	rBV	498	519	0.05%	0.006%
17	3.800	444	445	450	rVB2	661	595	0.06%	0.007%
18	3.861	450	455	456	rBV3	306	455	0.05%	0.005%
19	3.940	464	468	469	rBV	594	655	0.07%	0.008%
20	3.989	472	476	477	rBV	430	472	0.05%	0.006%
21	4.105	493	495	497	rBV2	518	422	0.04%	0.005%
22	4.136	497	500	502	rBV4	520	587	0.06%	0.007%
23	4.190	507	509	511	rBV2	422	412	0.04%	0.005%
24	4.489	547	558	575	rBV2	161277	517064	53.88%	6.124%
25	4.867	619	620	622	rVB	709	396	0.04%	0.005%
26	4.891	622	624	627	rBV2	411	649	0.07%	0.008%
27	5.074	641	654	668	rBV2	124536	391282	40.77%	4.635%
28	5.404	702	708	716	rBV6	1023	2689	0.28%	0.032%
29	5.495	719	723	724	rBV2	512	515	0.05%	0.006%
30	5.568	727	735	744	rVB6	1655	4849	0.51%	0.057%
31	5.983	791	803	819	rVV2	326109	959646	100.00%	11.366%
32	6.129	825	827	831	rVB3	612	680	0.07%	0.008%
33	6.349	861	863	865	rBV2	431	423	0.04%	0.005%
34	6.489	884	886	889	rVB3	543	506	0.05%	0.006%
35	6.775	923	933	945	rBV	298835	727564	75.82%	8.618%
36	7.129	982	991	1003	rBV5	11929	32674	3.40%	0.387%

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

37	7.318	1012	1022	1037	rVV	199389	437529	45.59%	5.182%
38	7.726	1087	1089	1091	rBV2	333	407	0.04%	0.005%
39	7.793	1094	1100	1101	rVB3	459	787	0.08%	0.009%
40	7.812	1101	1103	1106	rBV2	545	704	0.07%	0.008%
41	7.848	1108	1109	1111	rVB2	598	391	0.04%	0.005%
42	8.062	1141	1144	1146	rVB2	447	416	0.04%	0.005%
43	8.208	1162	1168	1169	rBV2	482	827	0.09%	0.010%
44	8.330	1179	1188	1197	rBV	129134	212522	22.15%	2.517%
45	8.482	1211	1213	1220	rBV6	901	1654	0.17%	0.020%
46	8.531	1220	1221	1225	rVB2	625	548	0.06%	0.006%
47	8.653	1235	1241	1250	rBV	444657	709016	73.88%	8.398%
48	8.958	1285	1291	1300	rBV	95806	142098	14.81%	1.683%
49	9.086	1310	1312	1316	rBV4	586	808	0.08%	0.010%
50	9.183	1326	1328	1330	rVV2	633	529	0.06%	0.006%
51	9.281	1340	1344	1349	rVB4	3018	4479	0.47%	0.053%
52	9.391	1356	1362	1377	rBV	469725	642127	66.91%	7.606%
53	9.714	1412	1415	1418	rBV2	594	491	0.05%	0.006%
54	9.824	1431	1433	1438	rVB2	548	560	0.06%	0.007%
55	10.061	1466	1472	1480	rBV	600348	836355	87.15%	9.906%
56	10.244	1500	1502	1505	rVB	554	431	0.04%	0.005%
57	10.305	1511	1512	1517	rVB3	1344	1382	0.14%	0.016%
58	10.348	1517	1519	1521	rBV	664	648	0.07%	0.008%
59	10.519	1544	1547	1549	rBV2	689	620	0.06%	0.007%
60	10.756	1584	1586	1587	rBV	470	395	0.04%	0.005%
61	10.829	1597	1598	1600	rVB2	691	392	0.04%	0.005%
62	10.872	1600	1605	1606	rBV	548	791	0.08%	0.009%
63	11.025	1628	1630	1633	rBV3	670	750	0.08%	0.009%
64	11.098	1636	1642	1645	rBV4	540	1374	0.14%	0.016%
65	11.195	1653	1658	1665	rBV	378891	486767	50.72%	5.765%
66	11.372	1686	1687	1689	rBV2	517	388	0.04%	0.005%
67	11.421	1694	1695	1697	rBV	558	391	0.04%	0.005%
68	11.445	1697	1699	1701	rVV3	569	426	0.04%	0.005%
69	11.482	1701	1705	1707	rVV	771	853	0.09%	0.010%
70	11.549	1712	1716	1718	rBV2	525	708	0.07%	0.008%
71	11.720	1742	1744	1746	rBV3	615	484	0.05%	0.006%
72	11.823	1758	1761	1762	rVB2	516	486	0.05%	0.006%
73	11.909	1772	1775	1780	rBV3	431	793	0.08%	0.009%
74	11.969	1783	1785	1789	rBV2	422	566	0.06%	0.007%
75	12.024	1789	1794	1801	rBV	667287	828209	86.30%	9.810%
76	12.232	1823	1828	1830	rBV3	1669	2741	0.29%	0.032%

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Peak Location: TOP

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Peak separation: 5

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 Title : VOC Analysis

77	12.323	1838	1843	1851	rBV	593037	716100	74.62%	8.482%
78	12.500	1870	1872	1874	rBV2	405	501	0.05%	0.006%
79	12.768	1913	1916	1917	rBV2	640	595	0.06%	0.007%
80	12.981	1948	1951	1954	rVV2	375	579	0.06%	0.007%
81	13.469	2029	2031	2036	rBV3	436	643	0.07%	0.008%
82	13.561	2044	2046	2048	rBV	604	471	0.05%	0.006%
83	13.658	2060	2062	2064	rBV	504	396	0.04%	0.005%
84	13.859	2093	2095	2098	rBV3	485	474	0.05%	0.006%
85	13.987	2115	2116	2121	rVB3	558	556	0.06%	0.007%
86	14.030	2121	2123	2124	rBV	541	394	0.04%	0.005%
87	14.189	2147	2149	2151	rBV2	571	577	0.06%	0.007%
88	14.335	2171	2173	2175	rBV2	426	430	0.04%	0.005%
89	14.408	2183	2185	2187	rVB	775	583	0.06%	0.007%
90	14.585	2213	2214	2217	rBV2	520	543	0.06%	0.006%
91	14.920	2267	2269	2272	rBV2	597	647	0.07%	0.008%
92	15.060	2290	2292	2295	rBV2	643	600	0.06%	0.007%
93	15.134	2302	2304	2306	rVB2	746	405	0.04%	0.005%
94	15.554	2372	2373	2376	rBV2	801	750	0.08%	0.009%
95	16.274	2488	2491	2494	rBV4	734	824	0.09%	0.010%
96	16.335	2500	2501	2502	rBV	726	417	0.04%	0.005%
97	16.524	2530	2532	2535	rBV4	809	719	0.07%	0.009%
98	16.609	2545	2546	2549	rVB	1153	779	0.08%	0.009%
99	16.645	2549	2552	2553	rVB2	760	578	0.06%	0.007%
100	16.664	2553	2555	2556	rBV2	551	408	0.04%	0.005%

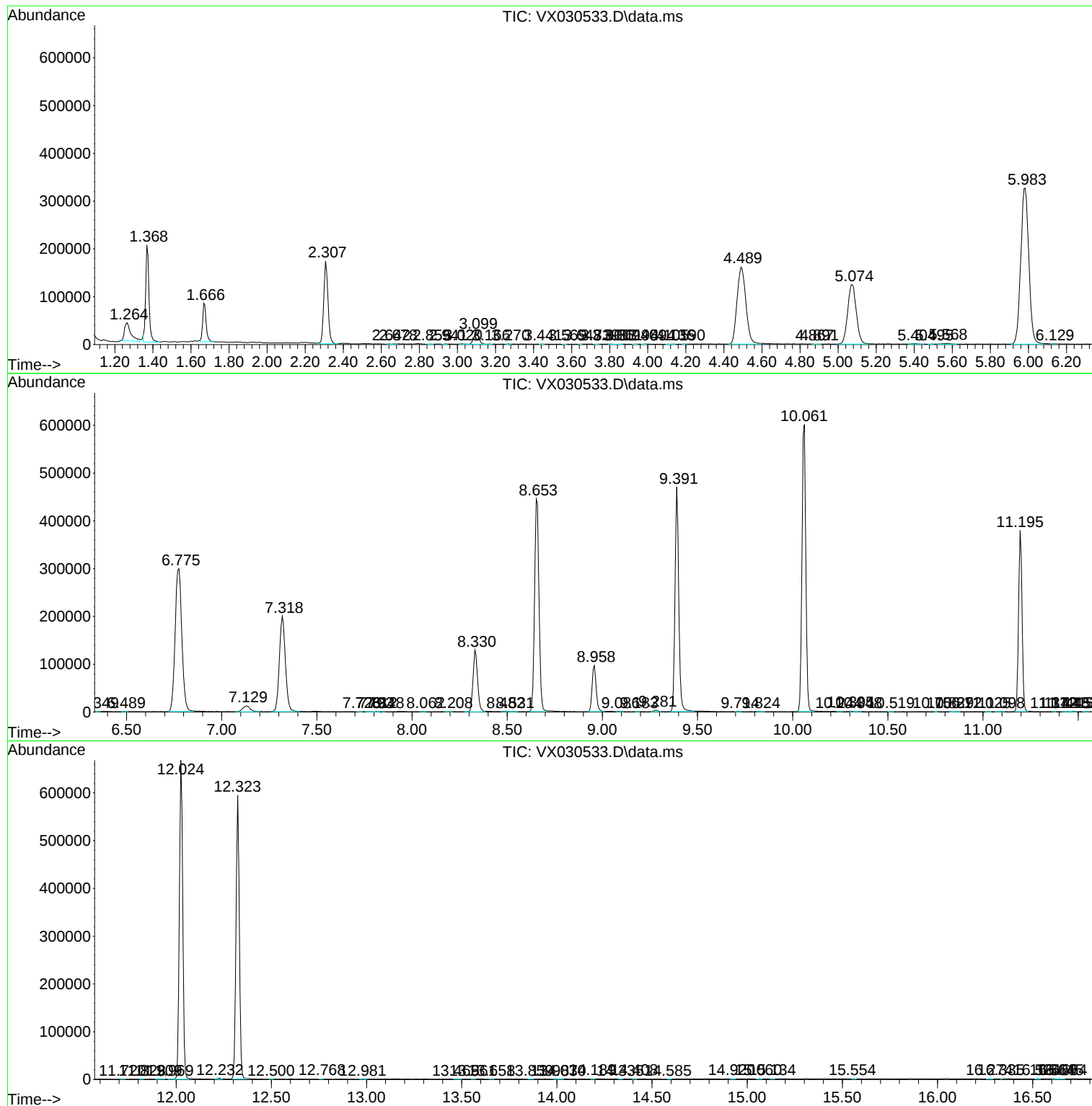
Sum of corrected areas: 8442796

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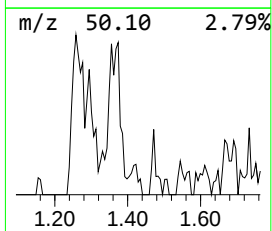
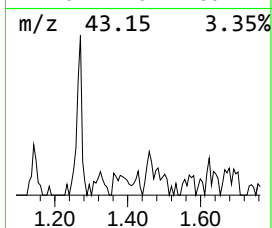
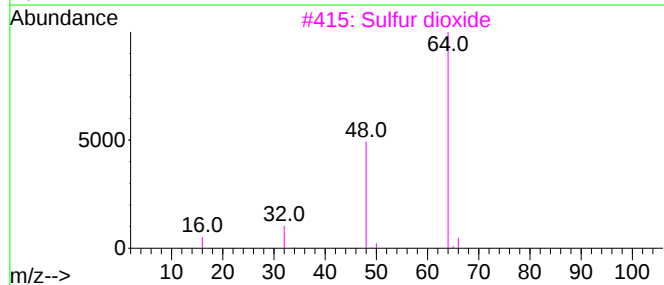
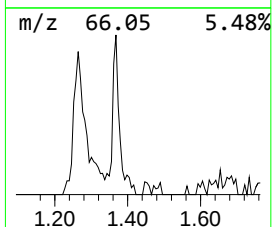
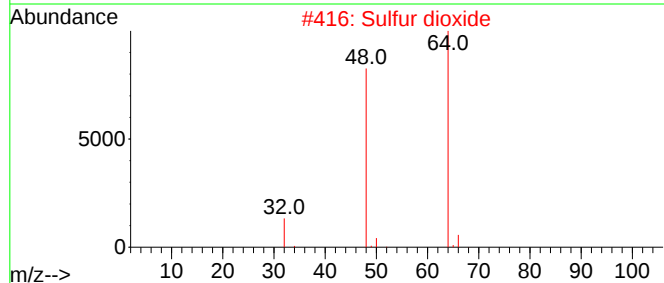
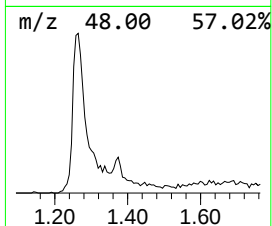
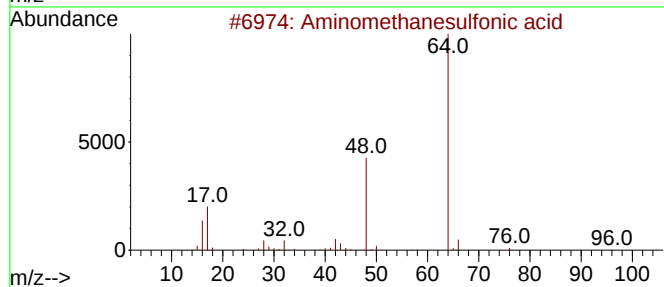
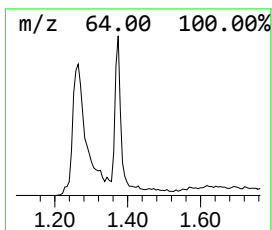
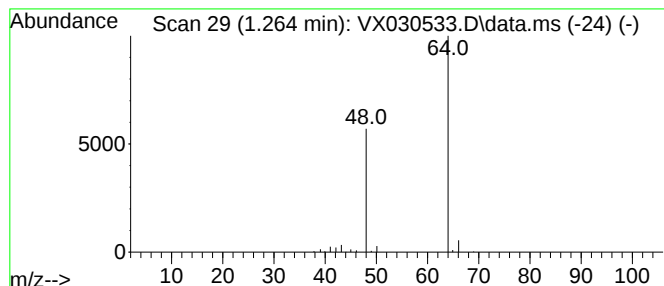
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	5.90 ug/L	85877	1,4-Difluorobenzene	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Sulfur dioxide	64	O2S	007446-09-5	83
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	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
Aminomethanesul...	1.264	5.9	ug/L	85877	1	6.775	727564	50.0