

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035149.D
 Acq On : 19 Apr 2023 01:43
 Operator : JC/MD
 Sample : 02397-13
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM5

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: VX035149.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	15	rBV2	6227	6714	0.33%	0.044%
2	1.252	23	27	42	rBV	95468	237016	11.73%	1.537%
3	1.368	43	46	57	rVB	246988	273913	13.55%	1.776%
4	1.672	92	96	106	rVB	176046	233840	11.57%	1.516%
5	2.306	193	200	209	rBV	441918	699254	34.60%	4.534%
6	2.654	255	257	258	rBV2	368	208	0.01%	0.001%
7	2.794	275	280	285	rVB4	853	1300	0.06%	0.008%
8	2.904	296	298	299	rBV	300	220	0.01%	0.001%
9	2.947	300	305	307	rBV2	976	1573	0.08%	0.010%
10	3.434	383	385	388	rVB2	233	233	0.01%	0.002%
11	3.471	388	391	393	rBV	446	533	0.03%	0.003%
12	3.514	395	398	401	rVV2	209	252	0.01%	0.002%
13	3.568	406	407	410	rVV	291	268	0.01%	0.002%
14	3.928	465	466	469	rVV2	287	238	0.01%	0.002%
15	3.971	472	473	476	rVV2	220	248	0.01%	0.002%
16	4.001	476	478	483	rVB3	605	856	0.04%	0.006%
17	4.221	511	514	515	rBV2	371	471	0.02%	0.003%
18	4.452	543	552	578	rBV	123583	369250	18.27%	2.394%
19	4.837	613	615	618	rBV3	297	353	0.02%	0.002%
20	4.897	623	625	627	rVB2	341	262	0.01%	0.002%
21	5.056	637	651	667	rBV	249717	770459	38.12%	4.996%
22	5.294	687	690	691	rBV2	363	352	0.02%	0.002%
23	5.385	703	705	706	rBV2	466	362	0.02%	0.002%
24	5.483	718	721	723	rBV2	387	354	0.02%	0.002%
25	5.556	725	733	735	rBV3	1054	1743	0.09%	0.011%
26	5.629	743	745	747	rBV2	324	256	0.01%	0.002%
27	5.763	765	767	771	rVB2	244	271	0.01%	0.002%
28	5.970	788	801	825	rBV2	664558	2021106	100.00%	13.106%
29	6.300	854	855	858	rVB3	554	509	0.03%	0.003%
30	6.330	858	860	863	rBV2	322	372	0.02%	0.002%
31	6.458	878	881	884	rVV3	315	497	0.02%	0.003%
32	6.537	892	894	898	rBV4	288	339	0.02%	0.002%
33	6.763	921	931	952	rBV	453660	1097251	54.29%	7.115%
34	7.031	973	975	977	rVB3	337	279	0.01%	0.002%
35	7.110	982	988	997	rVB7	2176	5214	0.26%	0.034%
36	7.306	1011	1020	1034	rBV	409743	901408	44.60%	5.845%

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 Title : VOC Analysis

37	7.458	1043	1045	1046	rBV2	451	347	0.02%	0.002%
38	7.476	1046	1048	1051	rVV3	961	1318	0.07%	0.009%
39	7.562	1060	1062	1064	rBV2	289	228	0.01%	0.001%
40	7.592	1064	1067	1068	rBV	398	507	0.03%	0.003%
41	7.793	1098	1100	1101	rBV	327	243	0.01%	0.002%
42	7.812	1101	1103	1105	rVV2	413	333	0.02%	0.002%
43	7.860	1109	1111	1113	rVV2	260	230	0.01%	0.001%
44	7.903	1116	1118	1119	rVV	505	389	0.02%	0.003%
45	7.940	1121	1124	1135	rVB5	1622	3590	0.18%	0.023%
46	8.055	1141	1143	1148	rBV3	192	246	0.01%	0.002%
47	8.098	1148	1150	1152	rVB2	342	244	0.01%	0.002%
48	8.196	1164	1166	1167	rBV2	322	235	0.01%	0.002%
49	8.324	1181	1187	1202	rBV	253851	414009	20.48%	2.685%
50	8.580	1222	1229	1233	rBV	11796	19735	0.98%	0.128%
51	8.647	1234	1240	1261	rVB	1053332	1645773	81.43%	10.672%
52	8.952	1284	1290	1302	rBV	174006	262559	12.99%	1.703%
53	9.104	1314	1315	1318	rVV2	630	365	0.02%	0.002%
54	9.135	1318	1320	1321	rVB	475	245	0.01%	0.002%
55	9.195	1328	1330	1334	rVB2	479	483	0.02%	0.003%
56	9.232	1334	1336	1338	rBV2	271	321	0.02%	0.002%
57	9.384	1355	1361	1381	rBV	573875	824181	40.78%	5.344%
58	9.653	1403	1405	1410	rVB4	819	944	0.05%	0.006%
59	9.708	1412	1414	1417	rVV2	317	243	0.01%	0.002%
60	9.781	1425	1426	1429	rVB3	293	266	0.01%	0.002%
61	9.958	1453	1455	1458	rVB2	579	666	0.03%	0.004%
62	9.982	1458	1459	1462	rBV	334	422	0.02%	0.003%
63	10.055	1465	1471	1487	rVV2	902997	1459393	72.21%	9.464%
64	10.738	1582	1583	1586	rBV2	291	241	0.01%	0.002%
65	10.866	1602	1604	1607	rBV3	976	868	0.04%	0.006%
66	11.067	1635	1637	1638	rBV	371	297	0.01%	0.002%
67	11.189	1652	1657	1670	rBV	672290	860349	42.57%	5.579%
68	11.488	1704	1706	1708	rVB2	436	294	0.01%	0.002%
69	11.591	1719	1723	1725	rBV3	316	427	0.02%	0.003%
70	11.616	1725	1727	1728	rBV	395	247	0.01%	0.002%
71	11.677	1735	1737	1740	rVB2	446	562	0.03%	0.004%
72	11.707	1740	1742	1745	rBV2	1090	1148	0.06%	0.007%
73	11.969	1781	1785	1789	rBV	37387	47520	2.35%	0.308%
74	12.024	1789	1794	1804	rVB2	845708	1297186	64.18%	8.412%
75	12.225	1823	1827	1831	rBV6	2057	3513	0.17%	0.023%
76	12.323	1837	1843	1851	rBV2	1013737	1501495	74.29%	9.737%

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 Title : VOC Analysis

77	12.658	1896	1898	1901	rVB3	372	389	0.02%	0.003%
78	12.689	1901	1903	1905	rBV	321	233	0.01%	0.002%
79	12.744	1909	1912	1913	rBV2	388	341	0.02%	0.002%
80	12.908	1936	1939	1940	rBV	557	561	0.03%	0.004%
81	12.969	1947	1949	1952	rBV2	320	416	0.02%	0.003%
82	13.055	1960	1963	1964	rBV2	503	517	0.03%	0.003%
83	13.116	1970	1973	1977	rBV2	1342	1534	0.08%	0.010%
84	13.213	1987	1989	1991	rVB	488	308	0.02%	0.002%
85	13.244	1991	1994	1995	rBV2	336	371	0.02%	0.002%
86	13.317	2004	2006	2009	rBV2	287	246	0.01%	0.002%
87	13.475	2030	2032	2036	rVB3	386	383	0.02%	0.002%
88	13.542	2041	2043	2045	rBV2	375	339	0.02%	0.002%
89	13.585	2045	2050	2065	rBV	226674	301625	14.92%	1.956%
90	13.731	2072	2074	2078	rVB3	538	536	0.03%	0.003%
91	13.774	2078	2081	2086	rBV4	540	820	0.04%	0.005%
92	13.878	2096	2098	2100	rBV2	384	441	0.02%	0.003%
93	13.963	2107	2112	2118	rVB	40723	54512	2.70%	0.353%
94	14.042	2123	2125	2127	rBV	332	278	0.01%	0.002%
95	14.256	2158	2160	2161	rBV2	346	238	0.01%	0.002%
96	14.347	2172	2175	2177	rBV2	370	486	0.02%	0.003%
97	14.554	2208	2209	2210	rBV	419	211	0.01%	0.001%
98	14.786	2240	2247	2252	rVB2	14211	20905	1.03%	0.136%
99	14.890	2262	2264	2266	rBV2	574	590	0.03%	0.004%
100	15.249	2318	2323	2331	rVB	38240	55467	2.74%	0.360%

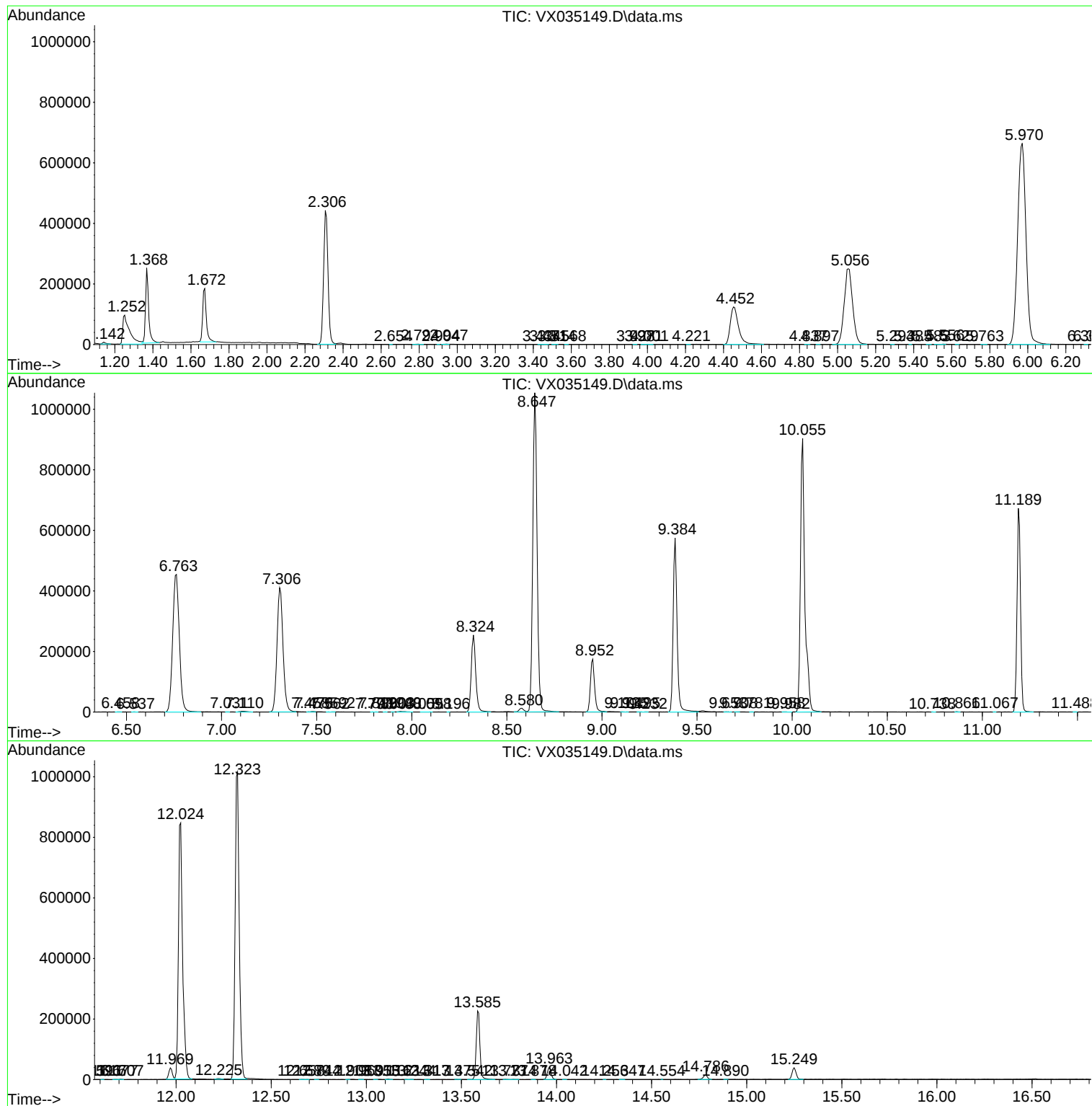
Sum of corrected areas: 15421183

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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



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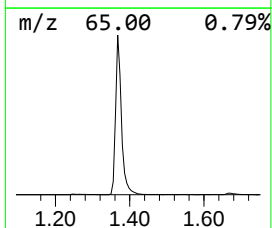
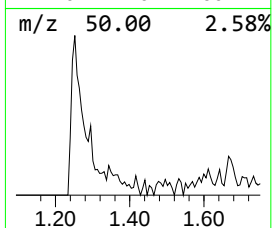
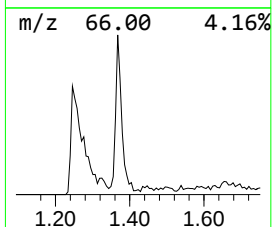
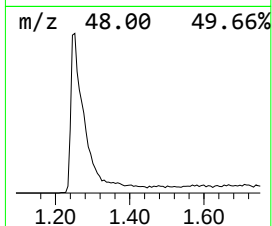
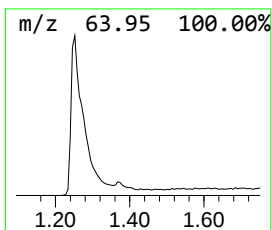
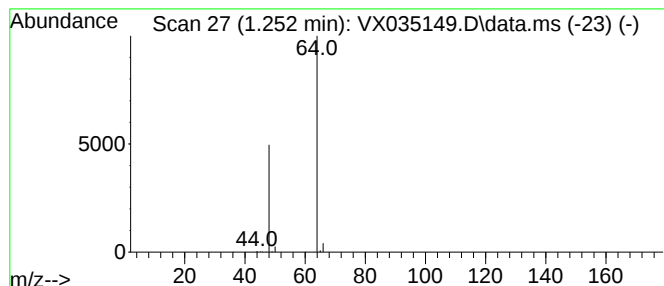
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	10.80 ug/L	237016	1,4-Difluorobenzene	6.763

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	10.8	ug/L	237016	1	6.763	1097250	50.0