

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
 Data File : VX025581.D
 Acq On : 07 Dec 2021 15:53
 Operator : JC/MD
 Sample : M4883-07ME
 Misc : 3.17g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9G3ME

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	43	rVB3	4660	13666	4.15%	0.486%
2	1.368	43	46	55	rVB	33296	38935	11.83%	1.384%
3	1.557	69	77	79	rBV3	3187	7516	2.28%	0.267%
4	1.648	89	92	98	rVB	20041	23820	7.24%	0.847%
5	2.276	189	195	206	rBV	62099	105745	32.12%	3.759%
6	2.953	298	306	322	rBV2	8030	23104	7.02%	0.821%
7	3.422	380	383	387	rVB3	216	286	0.09%	0.010%
8	4.282	519	524	532	rVB4	1126	2743	0.83%	0.097%
9	4.501	549	560	586	rBV2	13655	67897	20.62%	2.413%
10	5.068	641	653	669	rBV	41411	132612	40.28%	4.714%
11	5.458	711	717	725	rVB5	1157	2914	0.89%	0.104%
12	5.611	739	742	744	rBV2	251	260	0.08%	0.009%
13	5.970	789	801	817	rBV2	112934	329202	100.00%	11.701%
14	6.153	826	831	833	rBV4	434	754	0.23%	0.027%
15	6.251	842	847	852	rVB4	599	1090	0.33%	0.039%
16	6.355	856	864	865	rBV4	2481	4260	1.29%	0.151%
17	6.763	922	931	945	rBV	86738	226329	68.75%	8.045%
18	7.129	982	991	1002	rBV	55714	126313	38.37%	4.490%
19	7.312	1013	1021	1029	rBV	62634	149502	45.41%	5.314%
20	7.653	1076	1077	1081	rVV2	385	373	0.11%	0.013%
21	7.781	1091	1098	1100	rBV3	557	1127	0.34%	0.040%
22	7.952	1121	1126	1130	rBV2	943	1701	0.52%	0.060%
23	8.275	1174	1179	1182	rBV3	360	665	0.20%	0.024%
24	8.330	1182	1188	1202	rVV	32807	60459	18.37%	2.149%
25	8.598	1227	1232	1234	rBV2	1355	1958	0.59%	0.070%
26	8.653	1234	1241	1248	rVV	158779	269517	81.87%	9.580%
27	8.720	1248	1252	1257	rVV	4240	6366	1.93%	0.226%
28	8.818	1264	1268	1270	rBV3	397	437	0.13%	0.016%
29	8.848	1270	1273	1278	rVB2	623	777	0.24%	0.028%
30	8.958	1285	1291	1298	rVB	21299	38146	11.59%	1.356%
31	9.104	1311	1315	1318	rVB4	331	467	0.14%	0.017%
32	9.275	1340	1343	1347	rVB3	1158	1419	0.43%	0.050%
33	9.403	1357	1364	1375	rBV	87560	149292	45.35%	5.306%
34	9.561	1387	1390	1395	rVB	1439	2031	0.62%	0.072%
35	9.616	1395	1399	1403	rBV3	1213	1767	0.54%	0.063%
36	9.659	1403	1406	1410	rVV2	306	400	0.12%	0.014%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	9.714	1411	1415	1420	rVB3	714	1038	0.32%	0.037%
38	9.817	1428	1432	1437	rBV2	602	756	0.23%	0.027%
39	10.061	1466	1472	1481	rBV	177991	262880	79.85%	9.344%
40	10.195	1491	1494	1499	rVB2	772	1217	0.37%	0.043%
41	10.305	1507	1512	1517	rVV2	4867	6887	2.09%	0.245%
42	10.360	1518	1521	1525	rVB4	1005	1217	0.37%	0.043%
43	10.586	1554	1558	1562	rBV2	427	702	0.21%	0.025%
44	10.646	1564	1568	1573	rVB	4896	6365	1.93%	0.226%
45	10.762	1583	1587	1588	rBV3	589	848	0.26%	0.030%
46	10.781	1588	1590	1594	rVB2	1417	1442	0.44%	0.051%
47	10.860	1599	1603	1606	rBV3	698	892	0.27%	0.032%
48	10.963	1617	1620	1624	rVB	1165	1258	0.38%	0.045%
49	11.073	1635	1638	1640	rBV2	190	306	0.09%	0.011%
50	11.122	1640	1646	1649	rVV2	1498	2181	0.66%	0.078%
51	11.195	1653	1658	1667	rVV	118759	160334	48.70%	5.699%
52	11.305	1673	1676	1684	rVV3	1191	1818	0.55%	0.065%
53	11.384	1685	1689	1695	rVB3	1303	1965	0.60%	0.070%
54	11.457	1697	1701	1702	rBV2	666	693	0.21%	0.025%
55	11.482	1702	1705	1708	rVB	1050	1170	0.36%	0.042%
56	11.616	1723	1727	1733	rVB2	1192	1571	0.48%	0.056%
57	11.683	1736	1738	1740	rVV2	289	211	0.06%	0.007%
58	11.719	1740	1744	1746	rVV2	1077	1444	0.44%	0.051%
59	11.756	1746	1750	1754	rVV3	4977	6422	1.95%	0.228%
60	11.847	1758	1765	1767	rBV3	417	554	0.17%	0.020%
61	11.890	1769	1772	1776	rVV	651	860	0.26%	0.031%
62	11.933	1776	1779	1783	rVV4	962	1458	0.44%	0.052%
63	11.969	1783	1785	1789	rVB2	475	502	0.15%	0.018%
64	12.024	1789	1794	1802	rBV	211082	260829	79.23%	9.271%
65	12.091	1802	1805	1809	rVV2	1882	2793	0.85%	0.099%
66	12.152	1813	1815	1821	rVB2	1235	1396	0.42%	0.050%
67	12.225	1824	1827	1830	rBV3	452	581	0.18%	0.021%
68	12.268	1831	1834	1836	rVV2	478	480	0.15%	0.017%
69	12.323	1838	1843	1850	rVB	195289	248341	75.44%	8.827%
70	12.427	1856	1860	1864	rVB2	2136	2392	0.73%	0.085%
71	12.469	1865	1867	1874	rVB5	913	1028	0.31%	0.037%
72	12.536	1874	1878	1880	rBV3	430	663	0.20%	0.024%
73	12.719	1904	1908	1913	rBV4	290	572	0.17%	0.020%
74	12.927	1940	1942	1945	rVV3	461	458	0.14%	0.016%
75	12.969	1946	1949	1956	rVB3	829	1158	0.35%	0.041%
76	13.055	1961	1963	1967	rVB2	348	321	0.10%	0.011%

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 Title : VOC Analysis

77	13.103	1967	1971	1973	rBV	285	314	0.10%	0.011%
78	13.195	1985	1986	1989	rBV	189	205	0.06%	0.007%
79	13.268	1995	1998	2002	rVV3	2117	2564	0.78%	0.091%
80	13.323	2005	2007	2011	rBV2	201	297	0.09%	0.011%
81	13.384	2014	2017	2023	rVB2	1057	1276	0.39%	0.045%
82	13.579	2047	2049	2054	rVB	470	469	0.14%	0.017%
83	13.640	2057	2059	2061	rVB2	267	205	0.06%	0.007%
84	13.780	2074	2082	2088	rVB	4608	6556	1.99%	0.233%
85	13.847	2088	2093	2097	rBV4	1754	2108	0.64%	0.075%
86	14.042	2121	2125	2128	rBV2	1850	2210	0.67%	0.079%
87	14.109	2133	2136	2137	rBV2	433	359	0.11%	0.013%
88	14.140	2137	2141	2144	rVB2	685	920	0.28%	0.033%
89	14.170	2144	2146	2150	rBV2	223	217	0.07%	0.008%
90	14.506	2198	2201	2206	rVV4	379	679	0.21%	0.024%
91	14.640	2216	2223	2226	rBV2	2783	3895	1.18%	0.138%
92	14.670	2226	2228	2234	rVB2	578	627	0.19%	0.022%
93	14.755	2239	2242	2244	rVV2	1342	1683	0.51%	0.060%
94	14.780	2244	2246	2250	rVV	2792	3248	0.99%	0.115%
95	14.853	2254	2258	2261	rVB2	309	453	0.14%	0.016%
96	15.018	2282	2285	2287	rBV3	193	319	0.10%	0.011%
97	15.127	2301	2303	2305	rBV	294	324	0.10%	0.012%
98	15.213	2314	2317	2320	rVB4	807	812	0.25%	0.029%
99	15.493	2358	2363	2367	rVB5	495	895	0.27%	0.032%
100	15.615	2380	2383	2387	rBV4	698	957	0.29%	0.034%

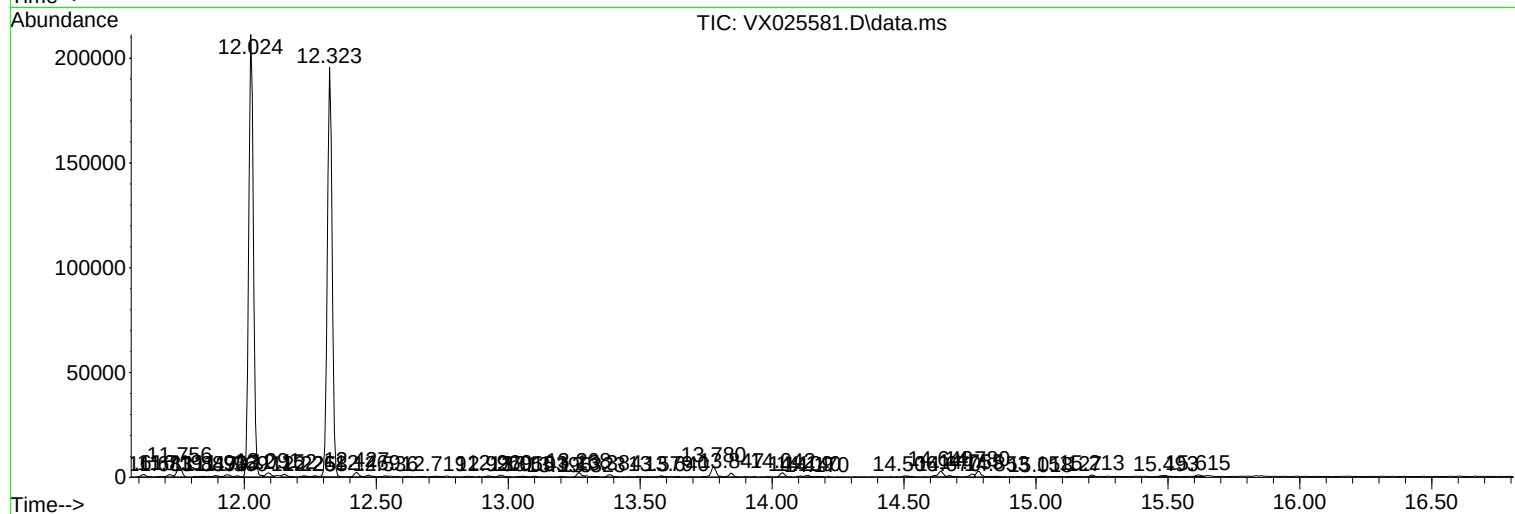
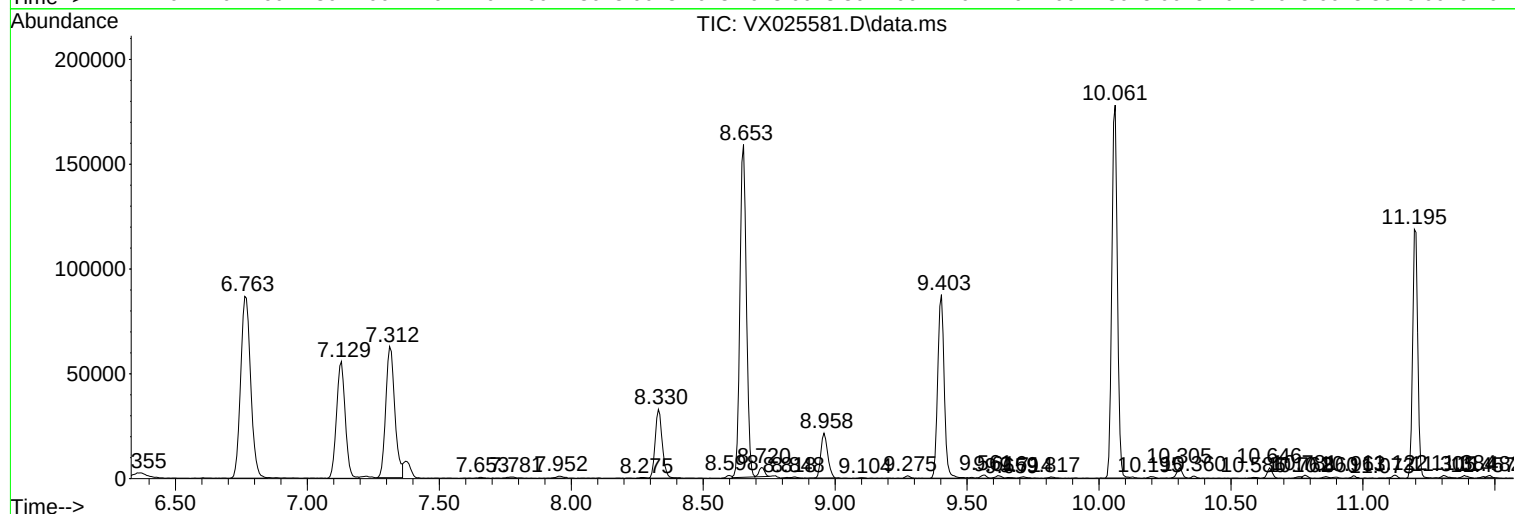
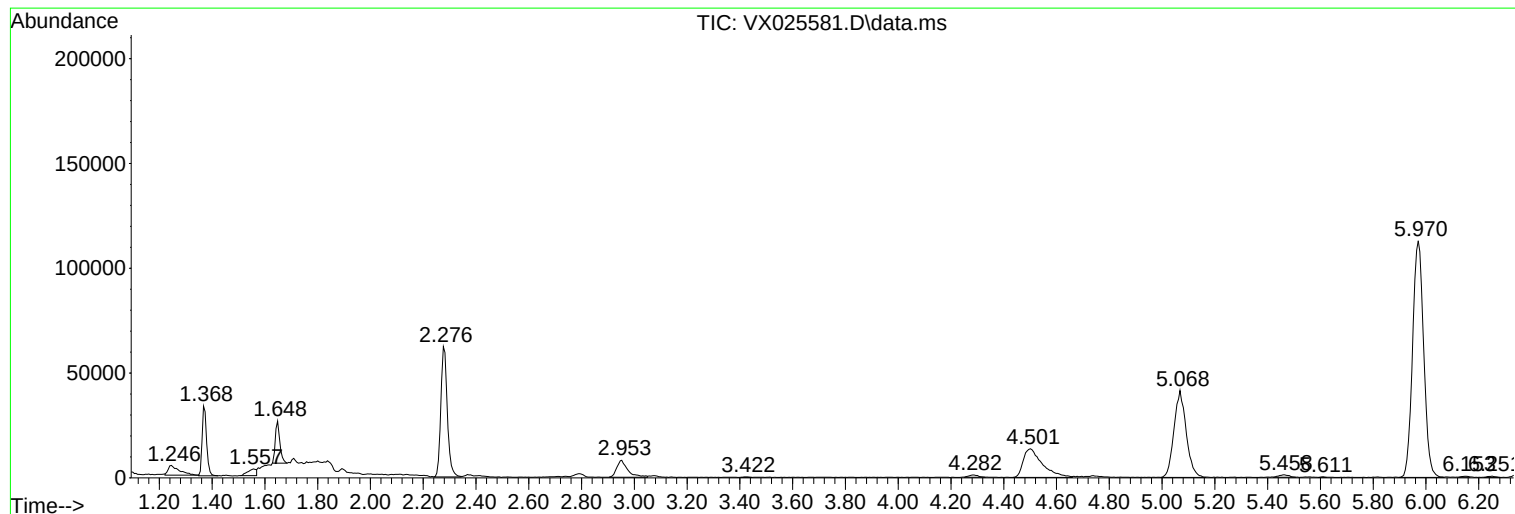
Sum of corrected areas: 2813445

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Instrument :
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ClientSampleId :
EW9G3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



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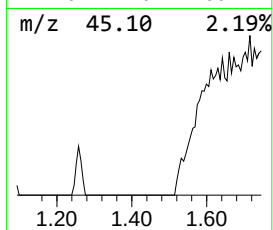
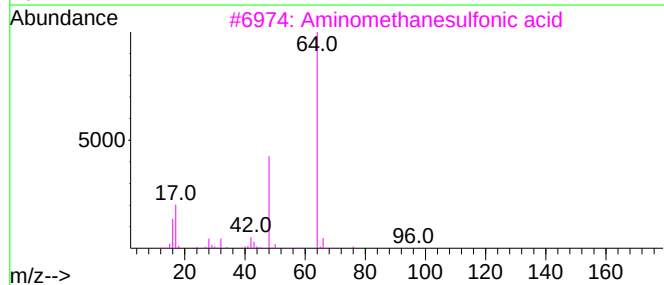
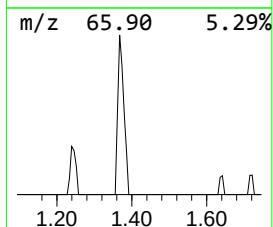
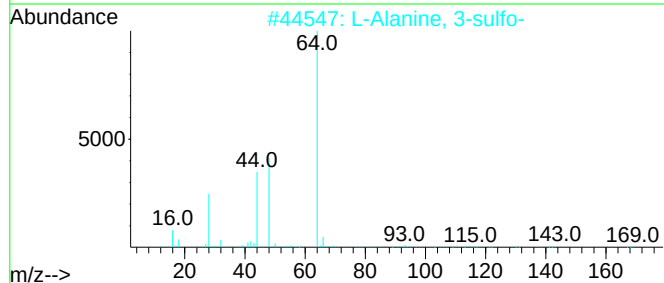
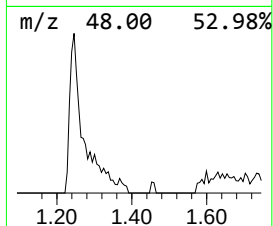
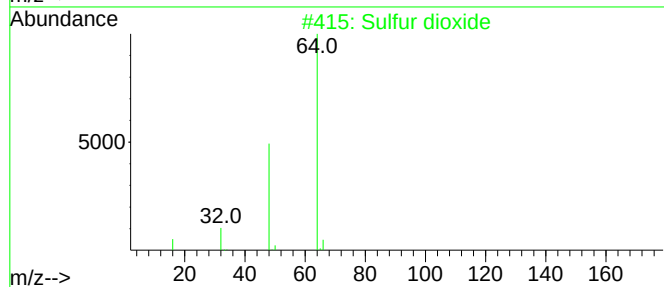
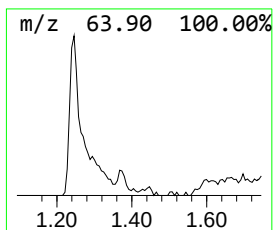
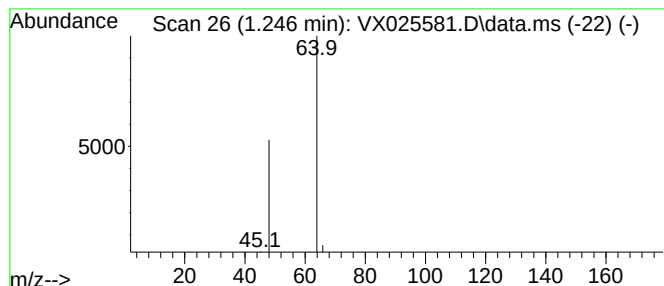
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	3.02 ug/L	13666	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	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	1.246	3.0	ug/L	13666	1	6.763	226329	50.0