

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072724\
 Data File : VX042581.D
 Acq On : 25 Jul 2024 20:51
 Operator : JC/MD
 Sample : P3334-21
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20M6

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\SFAMXML070324WMA.M

Title : VOC Analysis

Signal : TIC: VX042581.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	7	9	18	rVB	3983	5567	1.18%	0.157%
2	1.240	22	25	33	rBV	23988	32698	6.94%	0.921%
3	1.368	43	46	56	rBV	37329	46713	9.91%	1.315%
4	1.648	89	92	101	rVB	33433	42638	9.05%	1.200%
5	2.300	192	199	209	rBV	78004	123009	26.11%	3.463%
6	2.392	211	214	217	rBV2	724	900	0.19%	0.025%
7	2.453	222	224	227	rBV	215	173	0.04%	0.005%
8	2.483	227	229	230	rBV	140	118	0.03%	0.003%
9	2.508	230	233	238	rVB2	234	342	0.07%	0.010%
10	2.599	245	248	250	rVB2	163	196	0.04%	0.006%
11	2.630	250	253	254	rBV	156	99	0.02%	0.003%
12	2.709	263	266	268	rBV	158	170	0.04%	0.005%
13	2.782	273	278	280	rBV3	829	1134	0.24%	0.032%
14	2.947	297	305	311	rBV2	751	2088	0.44%	0.059%
15	3.099	326	330	334	rVB	349	377	0.08%	0.011%
16	3.190	344	345	347	rBV	153	122	0.03%	0.003%
17	3.221	349	350	355	rVB	127	160	0.03%	0.005%
18	3.282	358	360	363	rBV	130	184	0.04%	0.005%
19	3.434	383	385	386	rBV	337	172	0.04%	0.005%
20	3.538	401	402	405	rVB2	125	124	0.03%	0.003%
21	3.568	405	407	408	rBV2	122	92	0.02%	0.003%
22	3.587	408	410	412	rBV2	103	111	0.02%	0.003%
23	3.745	432	436	437	rBV	136	138	0.03%	0.004%
24	3.879	456	458	460	rVB2	145	106	0.02%	0.003%
25	3.916	460	464	469	rVB2	158	268	0.06%	0.008%
26	4.081	490	491	494	rBV2	143	185	0.04%	0.005%
27	4.294	523	526	527	rBV2	345	233	0.05%	0.007%
28	4.465	546	554	572	rBV	38793	116037	24.63%	3.267%
29	5.056	638	651	670	rBV	63103	188935	40.10%	5.319%
30	5.312	691	693	694	rBV	131	90	0.02%	0.003%
31	5.458	714	717	724	rVB3	323	644	0.14%	0.018%
32	5.513	724	726	727	rBV	122	85	0.02%	0.002%
33	5.562	732	734	735	rBV	209	110	0.02%	0.003%
34	5.964	789	800	823	rBV2	158378	471189	100.00%	13.265%
35	6.336	860	861	863	rBV	186	117	0.02%	0.003%
36	6.446	876	879	881	rVV	164	173	0.04%	0.005%

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 Title : VOC Analysis

37	6.580	900	901	904	rVB	137	125	0.03%	0.004%
38	6.623	907	908	911	rBV2	200	207	0.04%	0.006%
39	6.672	914	916	920	rVB2	122	134	0.03%	0.004%
40	6.757	922	930	948	rBV	134684	325335	69.05%	9.159%
41	6.958	961	963	966	rVB2	261	213	0.05%	0.006%
42	7.135	984	992	1000	rBV4	2768	6959	1.48%	0.196%
43	7.214	1002	1005	1006	rBV3	230	217	0.05%	0.006%
44	7.306	1012	1020	1039	rBV	95454	215673	45.77%	6.072%
45	7.488	1048	1050	1051	rBV	178	88	0.02%	0.002%
46	7.537	1056	1058	1059	rBV	144	135	0.03%	0.004%
47	7.854	1107	1110	1112	rBV2	123	141	0.03%	0.004%
48	8.122	1153	1154	1157	rVB	109	89	0.02%	0.003%
49	8.153	1157	1159	1160	rBV	116	106	0.02%	0.003%
50	8.190	1163	1165	1166	rBV	173	142	0.03%	0.004%
51	8.324	1181	1187	1202	rBV	54980	93150	19.77%	2.622%
52	8.525	1218	1220	1224	rBV2	129	201	0.04%	0.006%
53	8.574	1226	1228	1230	rVB	141	87	0.02%	0.002%
54	8.592	1230	1231	1234	rBV2	155	159	0.03%	0.004%
55	8.647	1234	1240	1249	rBV	225853	345209	73.26%	9.719%
56	8.952	1285	1290	1302	rBV	39289	60359	12.81%	1.699%
57	9.159	1322	1324	1327	rBV2	100	121	0.03%	0.003%
58	9.281	1340	1344	1348	rVB3	574	688	0.15%	0.019%
59	9.384	1356	1361	1376	rBV	166109	244940	51.98%	6.896%
60	9.604	1396	1397	1398	rBV	154	76	0.02%	0.002%
61	9.665	1405	1407	1408	rBV	130	92	0.02%	0.003%
62	9.756	1421	1422	1424	rVB	166	87	0.02%	0.002%
63	9.787	1424	1427	1429	rBV2	159	191	0.04%	0.005%
64	10.055	1465	1471	1487	rBV	267555	368684	78.25%	10.380%
65	10.195	1490	1494	1499	rVB2	774	1271	0.27%	0.036%
66	10.305	1508	1512	1519	rVB	1701	2251	0.48%	0.063%
67	10.592	1555	1559	1560	rBV2	152	183	0.04%	0.005%
68	10.646	1565	1568	1574	rVB	584	966	0.21%	0.027%
69	10.774	1587	1589	1593	rVB	144	165	0.04%	0.005%
70	10.963	1617	1620	1621	rBV	184	160	0.03%	0.005%
71	11.122	1643	1646	1647	rBV	140	136	0.03%	0.004%
72	11.189	1652	1657	1666	rBV	203665	259787	55.13%	7.314%
73	11.305	1674	1676	1679	rBV2	141	147	0.03%	0.004%
74	11.457	1698	1701	1704	rBV	253	327	0.07%	0.009%
75	11.616	1724	1727	1730	rVB2	119	158	0.03%	0.004%
76	11.726	1740	1745	1746	rBV2	111	189	0.04%	0.005%

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 Title : VOC Analysis

77	11.756	1746	1750	1755	rVB2	688	987	0.21%	0.028%
78	11.902	1772	1774	1776	rVV2	130	79	0.02%	0.002%
79	12.024	1789	1794	1808	rBV	225860	290532	61.66%	8.179%
80	12.219	1822	1826	1835	rVB	2639	3789	0.80%	0.107%
81	12.317	1837	1842	1857	rVV	218827	288873	61.31%	8.133%
82	12.859	1929	1931	1932	rBV	86	76	0.02%	0.002%
83	12.896	1935	1937	1940	rVV2	97	88	0.02%	0.002%
84	13.085	1965	1968	1969	rBV	114	149	0.03%	0.004%
85	13.183	1982	1984	1985	rBV	141	90	0.02%	0.003%
86	13.219	1988	1990	1992	rBV2	86	102	0.02%	0.003%
87	13.439	2022	2026	2027	rVV2	129	126	0.03%	0.004%
88	13.487	2032	2034	2036	rBV2	131	113	0.02%	0.003%
89	13.561	2044	2046	2048	rBV2	85	85	0.02%	0.002%
90	13.597	2050	2052	2053	rBV	93	84	0.02%	0.002%
91	13.725	2071	2073	2075	rVB	153	138	0.03%	0.004%
92	13.743	2075	2076	2079	rBV2	75	89	0.02%	0.003%
93	13.792	2079	2084	2086	rVV2	233	359	0.08%	0.010%
94	13.847	2090	2093	2096	rBV2	196	290	0.06%	0.008%
95	13.896	2100	2101	2105	rVB	111	113	0.02%	0.003%
96	14.060	2127	2128	2131	rVB2	120	93	0.02%	0.003%
97	14.384	2179	2181	2183	rBV2	193	155	0.03%	0.004%
98	14.512	2200	2202	2205	rBV	194	262	0.06%	0.007%
99	15.286	2327	2329	2331	rBV2	290	256	0.05%	0.007%
100	16.017	2447	2449	2451	rBV2	288	217	0.05%	0.006%

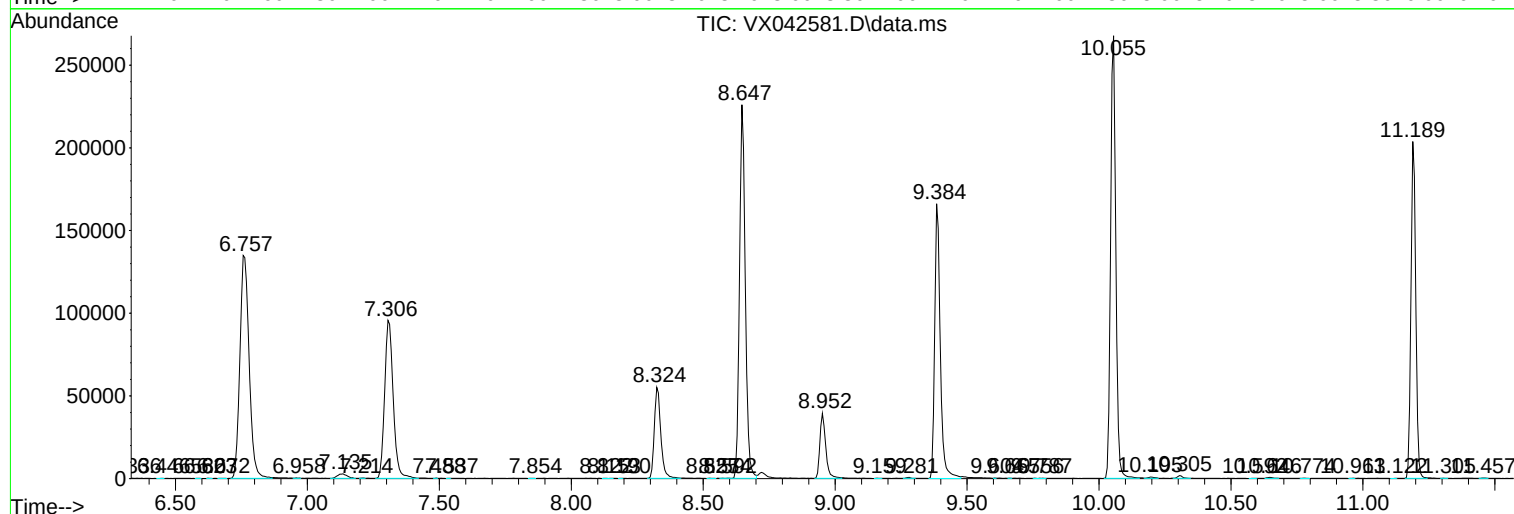
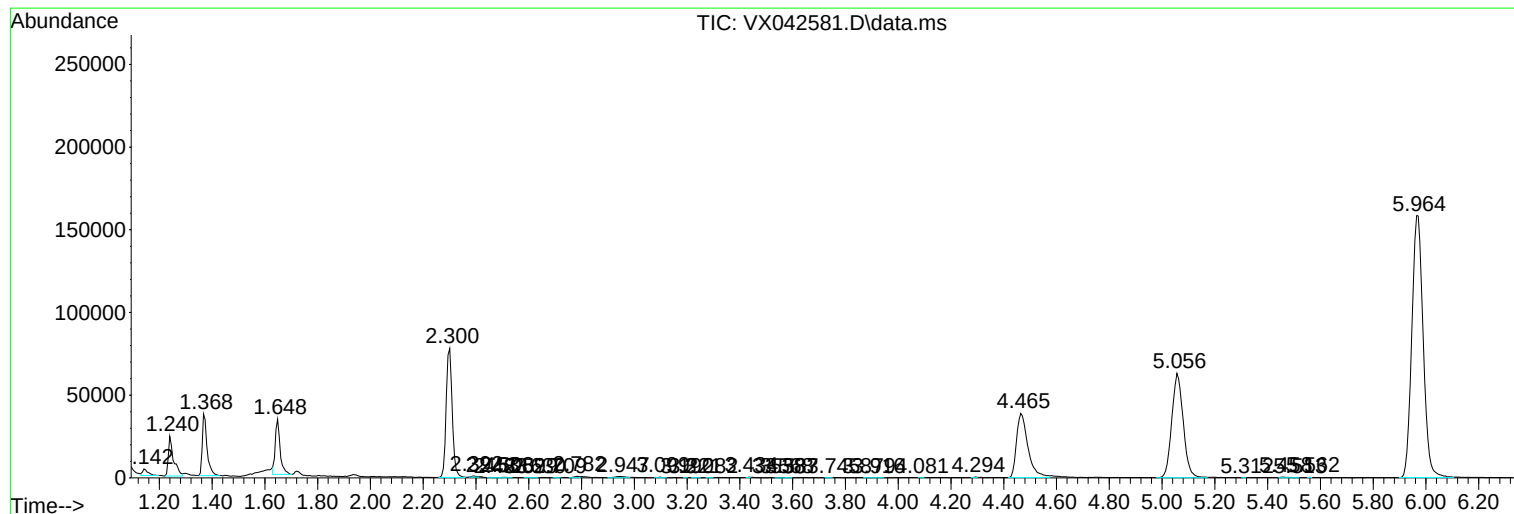
Sum of corrected areas: 3551990

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



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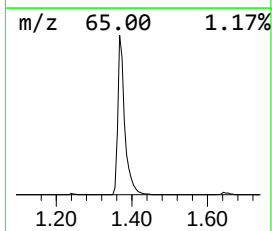
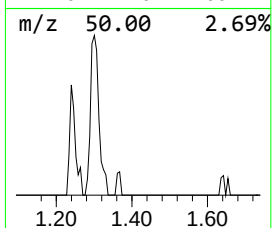
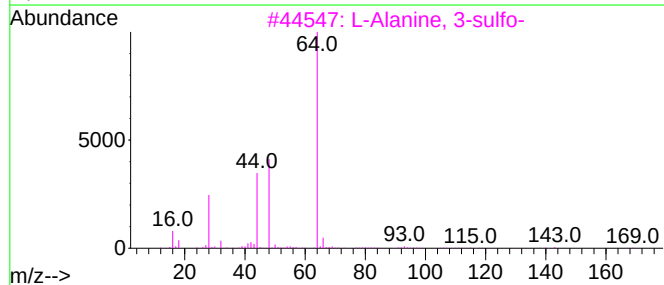
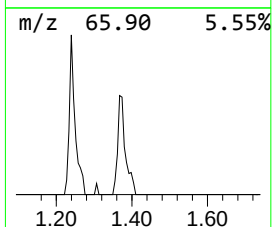
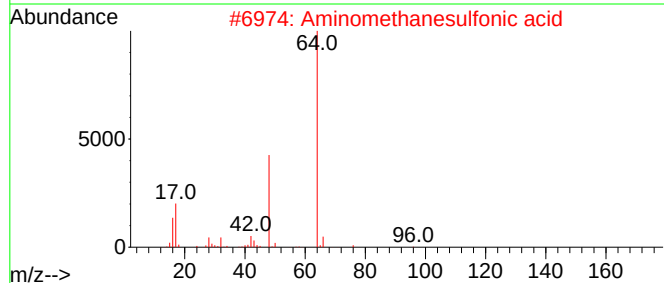
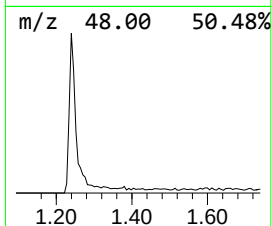
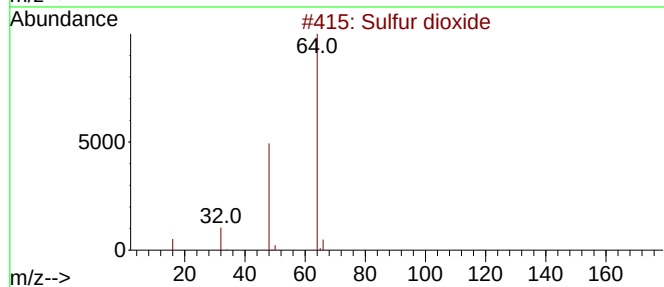
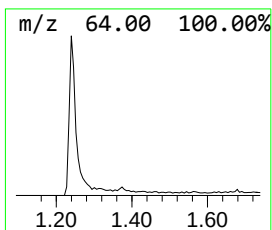
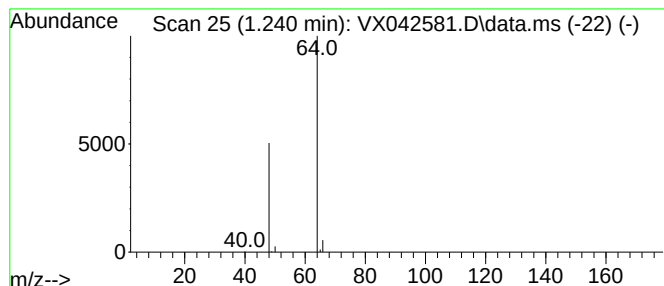
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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.
1.240	5.03 ug/L	32698	1,4-Difluorobenzene	6.757

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			Sulfur dioxide	64	O2S	007446-09-5	5



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	5.0	ug/L	32698	1	6.757	325335	50.0