

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072424\
 Data File : VX042498.D
 Acq On : 24 Jul 2024 01:45
 Operator : JC/MD
 Sample : P3327-32
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E20G3

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\SFAMXMLM070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042498.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	19	rVB	4855	7368	1.15%	0.149%
2	1.240	22	25	40	rVB2	13966	22722	3.54%	0.460%
3	1.368	43	46	57	rVV	62549	79581	12.39%	1.612%
4	1.453	57	60	64	rVB	2216	2389	0.37%	0.048%
5	1.648	88	92	102	rVB	50699	67288	10.47%	1.363%
6	2.300	192	199	209	rBV	125698	199784	31.10%	4.046%
7	2.392	209	214	224	rVB2	4021	9493	1.48%	0.192%
8	2.690	261	263	264	rBV	292	195	0.03%	0.004%
9	2.788	274	279	285	rBV2	958	1656	0.26%	0.034%
10	2.947	299	305	313	rBV	2390	5800	0.90%	0.117%
11	3.062	323	324	325	rVB	162	59	0.01%	0.001%
12	3.087	325	328	333	rBV3	950	1375	0.21%	0.028%
13	3.160	337	340	341	rBV	88	71	0.01%	0.001%
14	3.300	361	363	364	rBV	97	57	0.01%	0.001%
15	3.331	365	368	369	rBV	221	210	0.03%	0.004%
16	3.501	395	396	399	rVB2	155	129	0.02%	0.003%
17	3.532	399	401	402	rBV	161	101	0.02%	0.002%
18	3.587	409	410	411	rBV	184	90	0.01%	0.002%
19	3.605	411	413	415	rVV2	180	228	0.04%	0.005%
20	3.654	419	421	422	rVB	159	93	0.01%	0.002%
21	3.672	422	424	425	rBV	180	139	0.02%	0.003%
22	3.800	443	445	447	rBV	65	44	0.01%	0.001%
23	3.843	449	452	453	rBV	169	195	0.03%	0.004%
24	3.861	453	455	457	rBV2	199	172	0.03%	0.003%
25	3.916	461	464	466	rVB	100	93	0.01%	0.002%
26	4.263	519	521	523	rBV2	146	152	0.02%	0.003%
27	4.312	527	529	531	rBV2	138	102	0.02%	0.002%
28	4.465	546	554	573	rBV2	55005	187158	29.13%	3.790%
29	4.964	634	636	638	rBV	109	73	0.01%	0.001%
30	5.056	640	651	667	rBV2	81664	253502	39.46%	5.134%
31	5.446	713	715	716	rBV	159	91	0.01%	0.002%
32	5.489	720	722	724	rVB	183	92	0.01%	0.002%
33	5.629	744	745	747	rVB	117	77	0.01%	0.002%
34	5.964	789	800	825	rBV2	215917	642443	100.00%	13.011%
35	6.263	847	849	851	rVB	229	215	0.03%	0.004%
36	6.373	866	867	872	rVB2	198	147	0.02%	0.003%

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 Title : VOC Analysis

37	6.580	900	901	903	rVB	172	88	0.01%	0.002%
38	6.757	921	930	951	rBV	175033	424958	66.15%	8.606%
39	7.123	982	990	1001	rBV	150344	336491	52.38%	6.815%
40	7.305	1012	1020	1042	rVB	128347	288656	44.93%	5.846%
41	7.629	1071	1073	1076	rBV2	116	140	0.02%	0.003%
42	7.763	1093	1095	1098	rBV2	111	124	0.02%	0.003%
43	7.824	1103	1105	1108	rBV2	125	175	0.03%	0.004%
44	7.885	1114	1115	1116	rBV	126	50	0.01%	0.001%
45	7.964	1123	1128	1131	rBV3	421	775	0.12%	0.016%
46	8.324	1182	1187	1204	rBV	68251	114957	17.89%	2.328%
47	8.525	1217	1220	1226	rBV4	308	663	0.10%	0.013%
48	8.647	1234	1240	1251	rBV	297898	472591	73.56%	9.571%
49	8.952	1285	1290	1306	rBV	48277	73030	11.37%	1.479%
50	9.134	1317	1320	1321	rBV2	157	148	0.02%	0.003%
51	9.275	1339	1343	1349	rBV3	2643	4086	0.64%	0.083%
52	9.384	1356	1361	1379	rBV	194607	295207	45.95%	5.979%
53	9.701	1411	1413	1417	rVB4	392	365	0.06%	0.007%
54	9.787	1425	1427	1428	rBV	101	76	0.01%	0.002%
55	9.823	1431	1433	1434	rBV	142	94	0.01%	0.002%
56	9.976	1456	1458	1461	rVB	241	209	0.03%	0.004%
57	10.055	1465	1471	1483	rBV	319084	436142	67.89%	8.833%
58	10.195	1492	1494	1498	rVB3	528	669	0.10%	0.014%
59	10.274	1505	1507	1508	rBV	174	142	0.02%	0.003%
60	10.311	1508	1513	1519	rVB3	731	1125	0.18%	0.023%
61	10.488	1540	1542	1543	rBV	108	61	0.01%	0.001%
62	10.646	1565	1568	1572	rBV	337	466	0.07%	0.009%
63	10.695	1575	1576	1577	rBV	141	58	0.01%	0.001%
64	10.732	1581	1582	1583	rBV	140	59	0.01%	0.001%
65	10.799	1590	1593	1594	rBV2	143	125	0.02%	0.003%
66	10.902	1608	1610	1613	rBV2	91	95	0.01%	0.002%
67	10.963	1618	1620	1623	rVV	177	187	0.03%	0.004%
68	11.189	1652	1657	1668	rBV	236666	320020	49.81%	6.481%
69	11.390	1688	1690	1693	rVB2	164	135	0.02%	0.003%
70	11.457	1698	1701	1704	rVB	285	308	0.05%	0.006%
71	11.634	1728	1730	1731	rBV2	150	102	0.02%	0.002%
72	11.756	1749	1750	1753	rVB2	340	278	0.04%	0.006%
73	11.841	1763	1764	1766	rVB	137	80	0.01%	0.002%
74	11.866	1766	1768	1770	rBV	163	97	0.02%	0.002%
75	11.975	1785	1786	1788	rBV2	296	178	0.03%	0.004%
76	12.024	1788	1794	1805	rVV	247664	325778	50.71%	6.598%

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77	12.219	1822	1826	1835	rVB	4155	6383	0.99%	0.129%
78	12.317	1837	1842	1856	rBV	265341	345991	53.86%	7.007%
79	12.603	1888	1889	1892	rBV	185	100	0.02%	0.002%
80	12.652	1894	1897	1898	rBV	245	237	0.04%	0.005%
81	12.878	1931	1934	1935	rBV2	93	115	0.02%	0.002%
82	12.957	1945	1947	1948	rVB	150	75	0.01%	0.002%
83	13.122	1972	1974	1976	rBV	307	290	0.05%	0.006%
84	13.335	2007	2009	2012	rBB	111	106	0.02%	0.002%
85	13.408	2019	2021	2022	rBV	131	64	0.01%	0.001%
86	13.536	2040	2042	2044	rBV	132	109	0.02%	0.002%
87	13.597	2050	2052	2053	rVB	199	97	0.02%	0.002%
88	13.957	2109	2111	2117	rBV2	178	185	0.03%	0.004%
89	14.127	2136	2139	2147	rVB3	674	1115	0.17%	0.023%
90	14.182	2147	2148	2151	rBV2	260	251	0.04%	0.005%
91	14.536	2205	2206	2207	rBV	195	96	0.01%	0.002%
92	14.798	2247	2249	2251	rBV	237	216	0.03%	0.004%

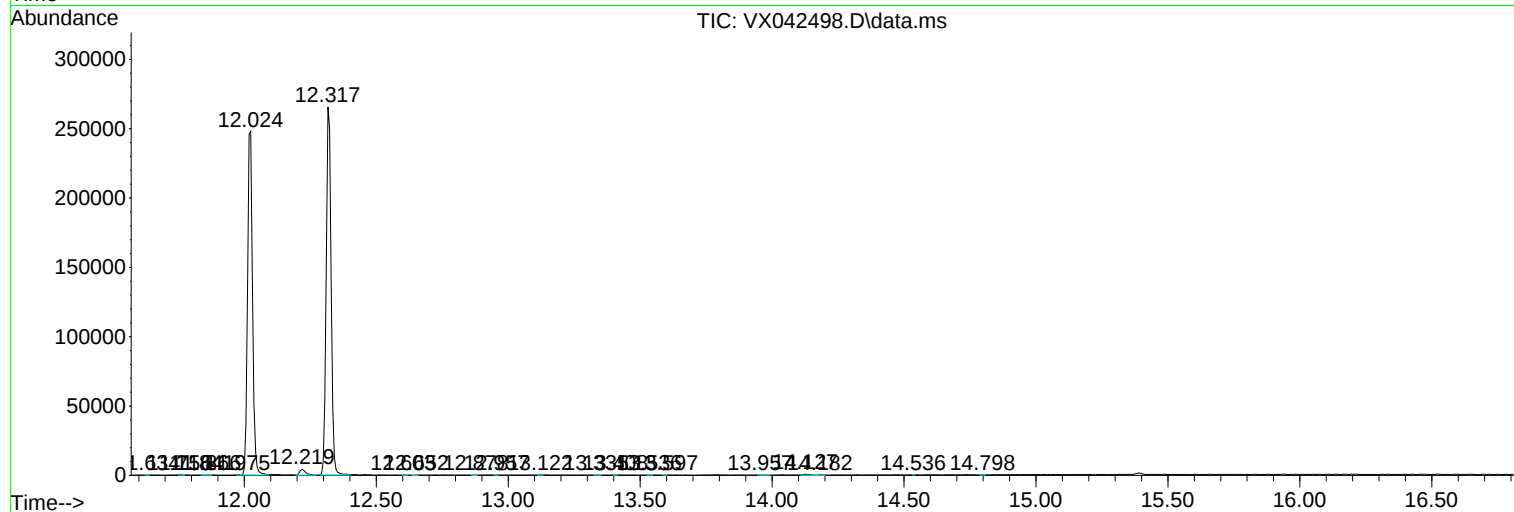
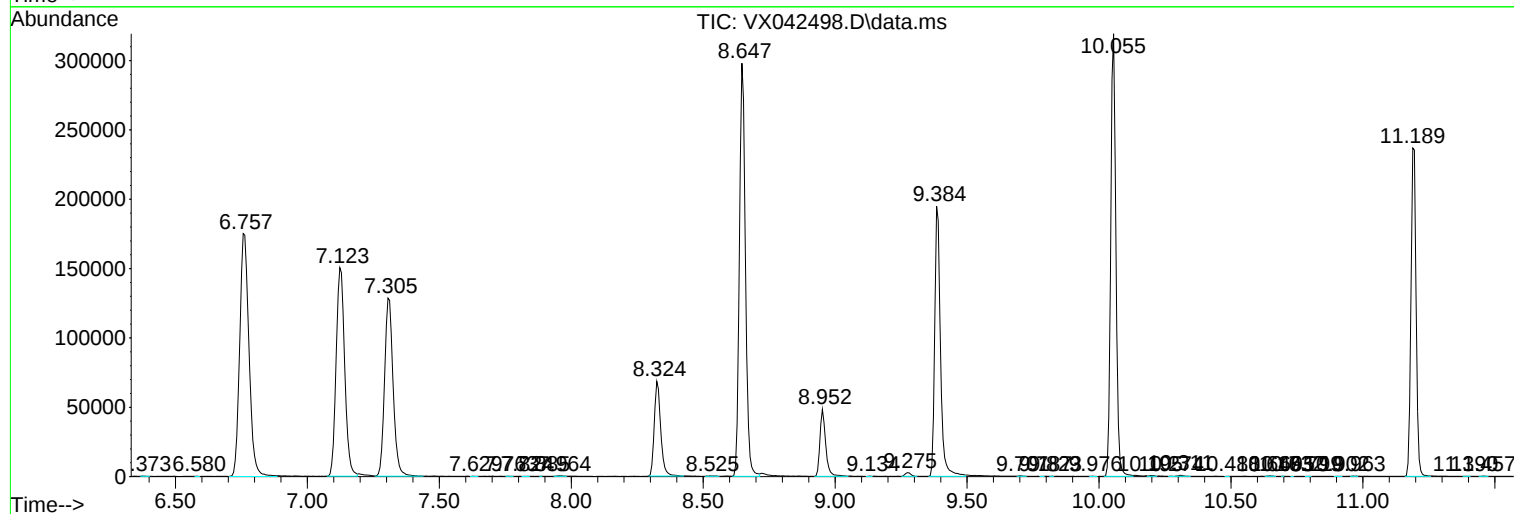
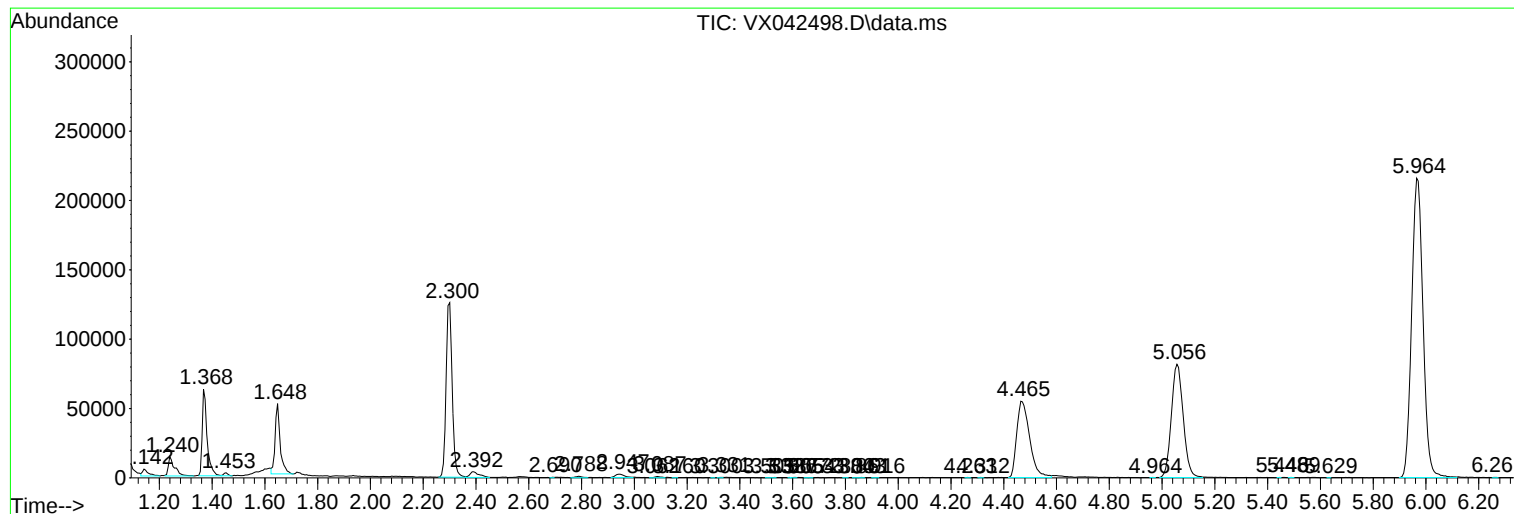
Sum of corrected areas: 4937802

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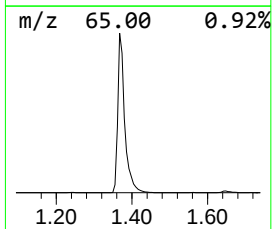
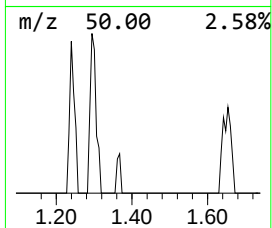
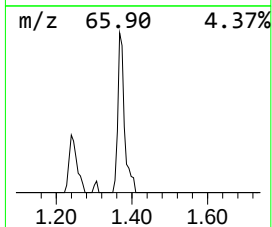
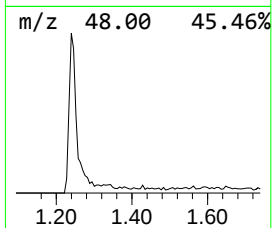
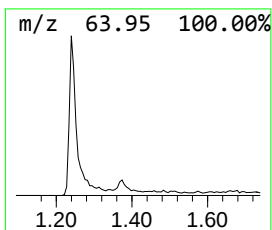
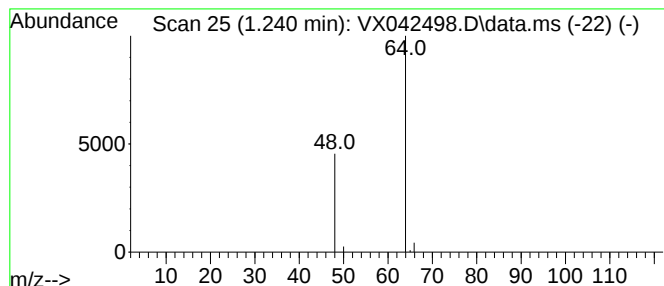
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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	2.67 ug/L	22722	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	2.7	ug/L	22722	1	6.757	424958	50.0