

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042782.D
 Acq On : 31 Jul 2024 18:44
 Operator : JC/MD
 Sample : P3398-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E08L2

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042782.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	16	rVB3	1283	1417	0.28%	0.039%
2	1.209	18	20	22	rBV	415	313	0.06%	0.009%
3	1.240	22	25	33	rBV	14184	19779	3.94%	0.541%
4	1.368	42	46	55	rBV	44357	56209	11.20%	1.538%
5	1.581	70	81	82	rBV3	2536	5890	1.17%	0.161%
6	1.648	89	92	100	rVB	26351	33824	6.74%	0.926%
7	2.056	155	159	160	rBV2	307	399	0.08%	0.011%
8	2.294	191	198	211	rBV	99217	157966	31.49%	4.323%
9	2.794	271	280	281	rBV4	948	1726	0.34%	0.047%
10	2.947	298	305	313	rVV2	1984	4599	0.92%	0.126%
11	3.123	331	334	336	rBB	205	220	0.04%	0.006%
12	3.453	386	388	392	rBB	232	281	0.06%	0.008%
13	3.751	434	437	440	rVV2	273	330	0.07%	0.009%
14	4.117	495	497	500	rVB	220	231	0.05%	0.006%
15	4.471	547	555	568	rBV	34705	100817	20.10%	2.759%
16	4.897	621	625	627	rBV	254	386	0.08%	0.011%
17	5.056	639	651	669	rBV	67320	204257	40.71%	5.590%
18	5.397	705	707	710	rVB	274	232	0.05%	0.006%
19	5.568	732	735	737	rBV	349	357	0.07%	0.010%
20	5.617	741	743	750	rVB2	227	362	0.07%	0.010%
21	5.970	787	801	818	rBV2	168860	501685	100.00%	13.730%
22	6.379	867	868	873	rVB	361	410	0.08%	0.011%
23	6.641	907	911	915	rBV	253	586	0.12%	0.016%
24	6.763	922	931	948	rBV2	124392	299399	59.68%	8.194%
25	7.019	969	973	975	rBV2	329	408	0.08%	0.011%
26	7.123	985	990	998	rBV4	700	1954	0.39%	0.053%
27	7.226	1004	1007	1008	rBV	320	313	0.06%	0.009%
28	7.245	1008	1010	1012	rVV2	334	354	0.07%	0.010%
29	7.312	1012	1021	1040	rVV	100006	225801	45.01%	6.180%
30	7.488	1048	1050	1053	rVB2	223	246	0.05%	0.007%
31	7.635	1072	1074	1076	rBV2	255	295	0.06%	0.008%
32	7.690	1080	1083	1084	rBV2	282	304	0.06%	0.008%
33	7.818	1099	1104	1105	rBV2	440	420	0.08%	0.011%
34	7.903	1115	1118	1120	rVB	241	279	0.06%	0.008%
35	7.933	1120	1123	1125	rBB2	211	254	0.05%	0.007%
36	8.226	1169	1171	1174	rVB2	225	244	0.05%	0.007%

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 Title : VOC Analysis

37	8.324	1181	1187	1197	rBV	59126	99228	19.78%	2.716%
38	8.531	1218	1221	1223	rVB2	263	224	0.04%	0.006%
39	8.647	1234	1240	1251	rBV	231716	389387	77.62%	10.657%
40	8.952	1285	1290	1301	rBV	44151	64475	12.85%	1.765%
41	9.281	1338	1344	1348	rBV	3351	5278	1.05%	0.144%
42	9.391	1356	1362	1381	rBV	157408	242129	48.26%	6.626%
43	9.653	1403	1405	1407	rBV	261	242	0.05%	0.007%
44	9.683	1407	1410	1412	rVV	260	241	0.05%	0.007%
45	9.744	1416	1420	1422	rBV2	191	267	0.05%	0.007%
46	9.951	1452	1454	1457	rVB	329	246	0.05%	0.007%
47	10.055	1465	1471	1488	rBV	249874	345823	68.93%	9.464%
48	10.207	1492	1496	1498	rBV4	256	361	0.07%	0.010%
49	10.311	1508	1513	1519	rBV3	522	1324	0.26%	0.036%
50	10.433	1530	1533	1536	rVV	337	297	0.06%	0.008%
51	10.659	1566	1570	1572	rVB2	886	1141	0.23%	0.031%
52	10.683	1572	1574	1576	rBV2	251	244	0.05%	0.007%
53	10.805	1593	1594	1597	rVB2	396	370	0.07%	0.010%
54	10.841	1597	1600	1602	rBV	287	295	0.06%	0.008%
55	10.963	1616	1620	1621	rBV2	389	455	0.09%	0.012%
56	11.189	1652	1657	1669	rVB	185696	252226	50.28%	6.903%
57	11.311	1673	1677	1684	rVB3	3446	4973	0.99%	0.136%
58	11.384	1684	1689	1692	rBB	199	340	0.07%	0.009%
59	11.421	1692	1695	1696	rBV	225	257	0.05%	0.007%
60	11.463	1699	1702	1704	rVB2	239	260	0.05%	0.007%
61	11.518	1704	1711	1712	rBV	267	458	0.09%	0.013%
62	11.652	1730	1733	1735	rBV	178	226	0.05%	0.006%
63	11.707	1739	1742	1745	rBV	182	256	0.05%	0.007%
64	11.847	1762	1765	1770	rVB2	344	506	0.10%	0.014%
65	11.914	1772	1776	1777	rBV2	284	379	0.08%	0.010%
66	11.969	1781	1785	1787	rBV2	204	284	0.06%	0.008%
67	12.024	1788	1794	1805	rBV	212699	281615	56.13%	7.707%
68	12.231	1825	1828	1834	rVB3	619	1044	0.21%	0.029%
69	12.323	1837	1843	1852	rBV	234194	312494	62.29%	8.552%
70	12.494	1870	1871	1875	rVB	265	234	0.05%	0.006%
71	12.762	1910	1915	1919	rBV2	1122	1480	0.30%	0.041%
72	12.853	1926	1930	1931	rBV2	466	503	0.10%	0.014%
73	12.866	1931	1932	1934	rVB2	602	249	0.05%	0.007%
74	12.926	1939	1942	1945	rBV2	265	366	0.07%	0.010%
75	13.018	1954	1957	1959	rBV2	272	392	0.08%	0.011%
76	13.091	1965	1969	1971	rBV	357	443	0.09%	0.012%

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 Title : VOC Analysis

77	13.384	2013	2017	2018	rBV2	258	338	0.07%	0.009%
78	13.457	2028	2029	2031	rVV	272	252	0.05%	0.007%
79	13.670	2062	2064	2067	rVB	282	313	0.06%	0.009%
80	13.713	2067	2071	2075	rBV2	174	327	0.07%	0.009%
81	13.780	2077	2082	2095	rVB	4948	7542	1.50%	0.206%
82	13.871	2095	2097	2099	rBV	353	268	0.05%	0.007%
83	14.085	2129	2132	2135	rBV2	167	226	0.05%	0.006%
84	14.127	2136	2139	2143	rVV	1851	2250	0.45%	0.062%
85	14.524	2202	2204	2207	rBV2	272	239	0.05%	0.007%
86	14.658	2223	2226	2228	rBV2	437	480	0.10%	0.013%
87	14.786	2245	2247	2249	rBV	291	229	0.05%	0.006%
88	14.963	2272	2276	2279	rBV	299	506	0.10%	0.014%
89	15.109	2298	2300	2302	rBV2	471	516	0.10%	0.014%
90	15.335	2335	2337	2340	rBV2	383	391	0.08%	0.011%
91	15.389	2342	2346	2351	rVV3	2153	3174	0.63%	0.087%
92	15.609	2379	2382	2383	rBV	310	346	0.07%	0.009%
93	15.847	2420	2421	2423	rVB	475	278	0.06%	0.008%
94	15.871	2423	2425	2427	rBV2	233	267	0.05%	0.007%
95	16.127	2465	2467	2468	rBV	383	249	0.05%	0.007%
96	16.231	2482	2484	2485	rBV	450	259	0.05%	0.007%
97	16.408	2510	2513	2516	rBV2	390	521	0.10%	0.014%
98	16.590	2541	2543	2546	rBV2	443	581	0.12%	0.016%
99	16.664	2551	2555	2556	rBV2	313	382	0.08%	0.010%
100	16.731	2564	2566	2572	rBV3	384	467	0.09%	0.013%

Sum of corrected areas: 3653960

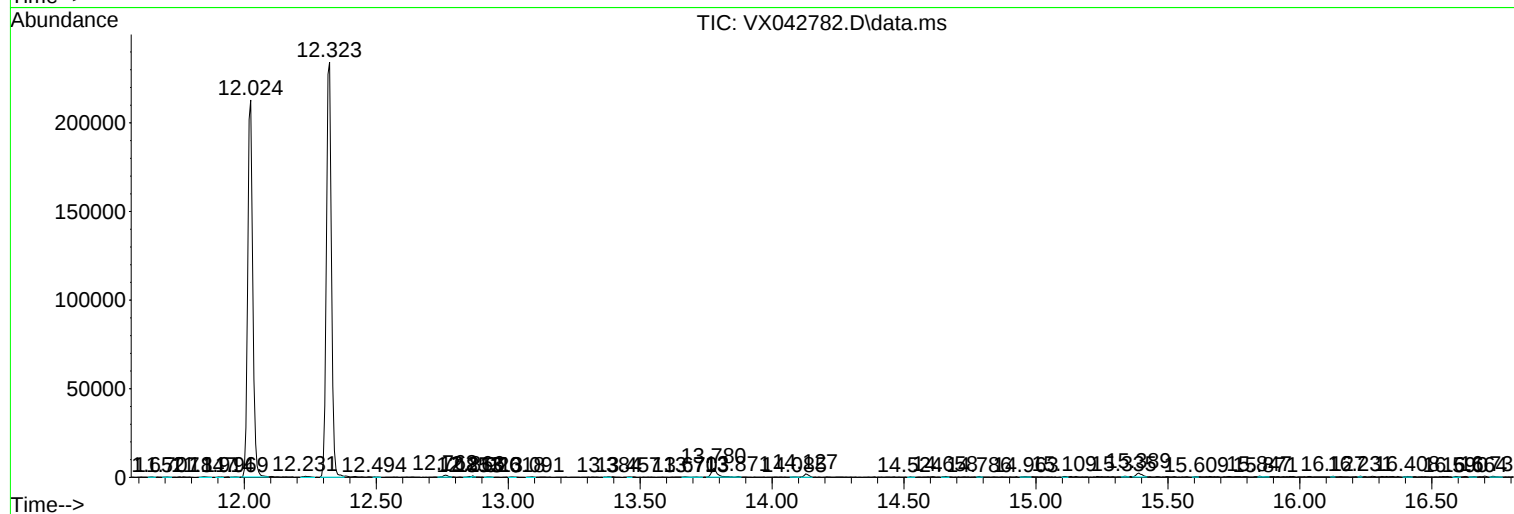
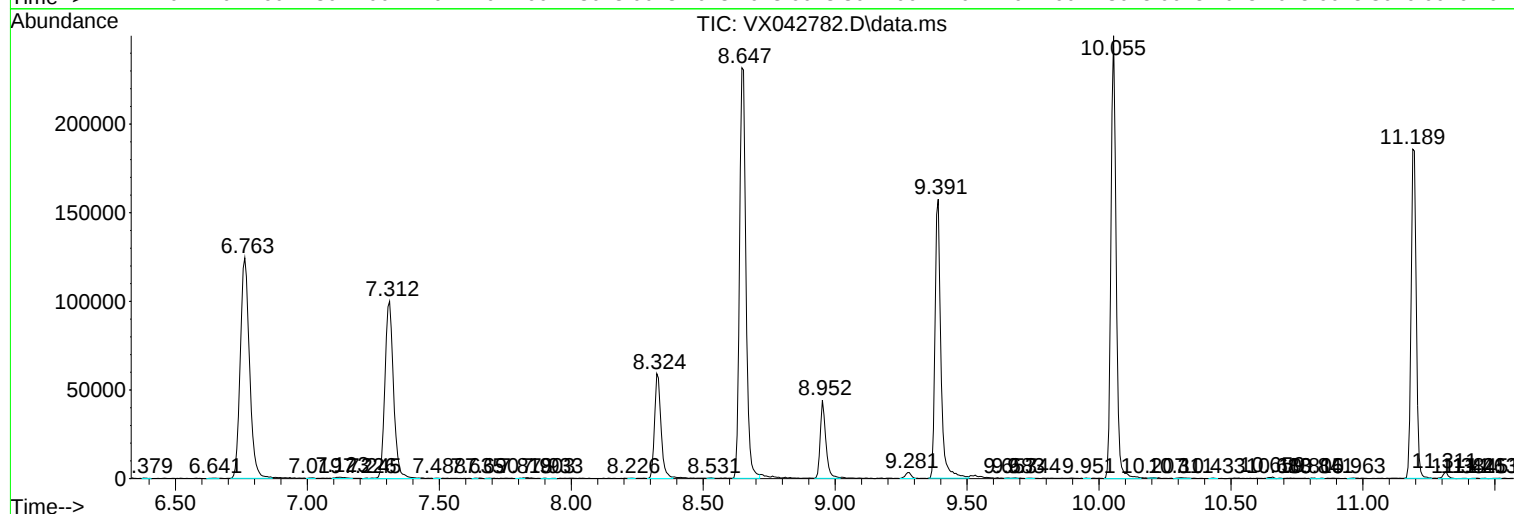
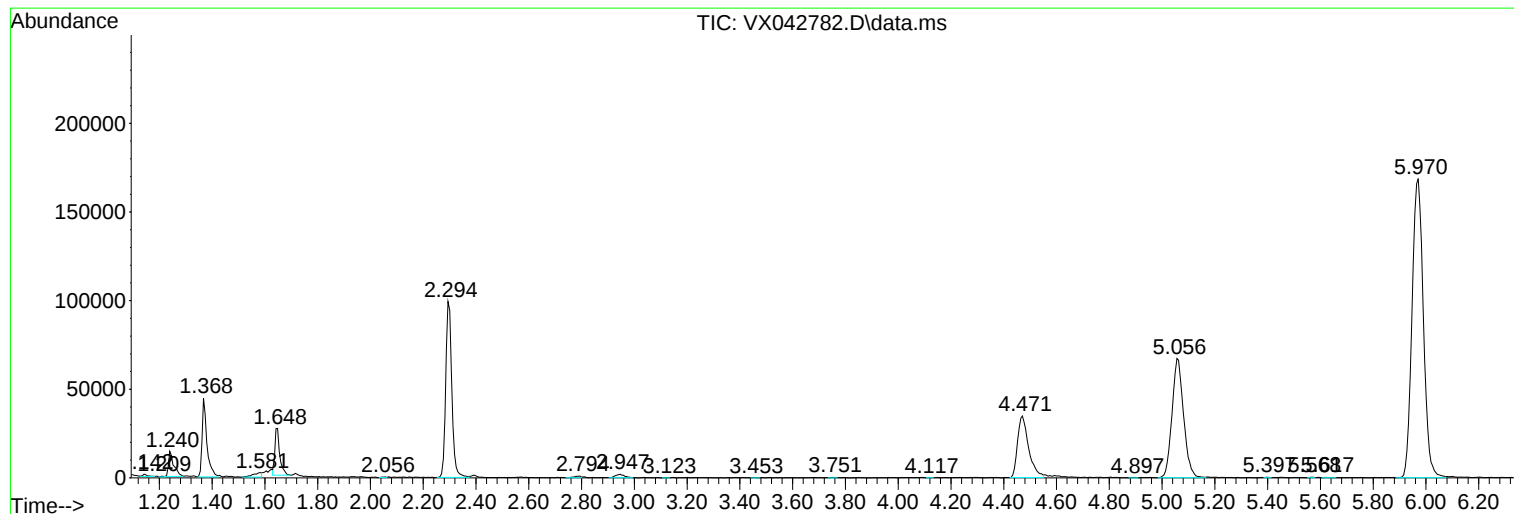
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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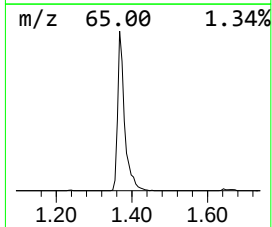
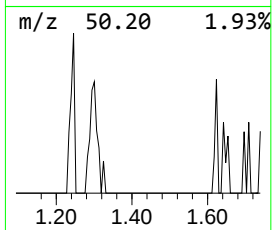
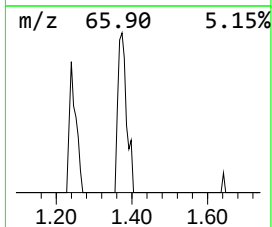
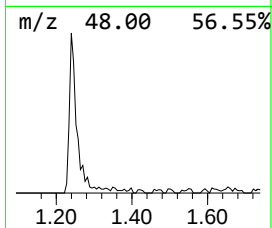
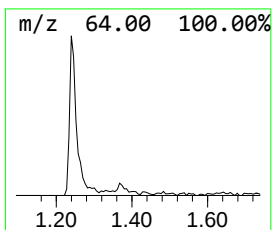
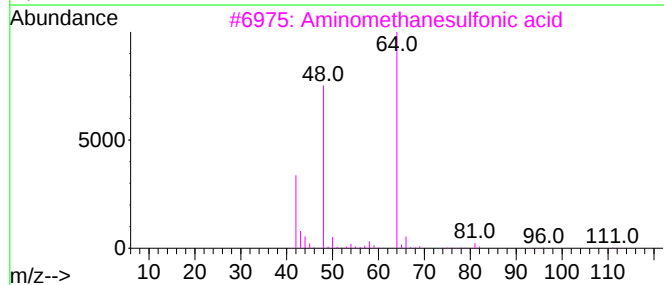
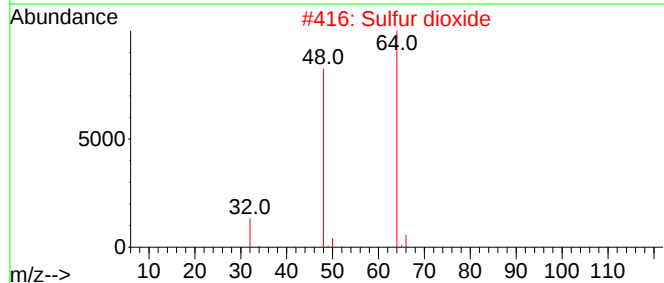
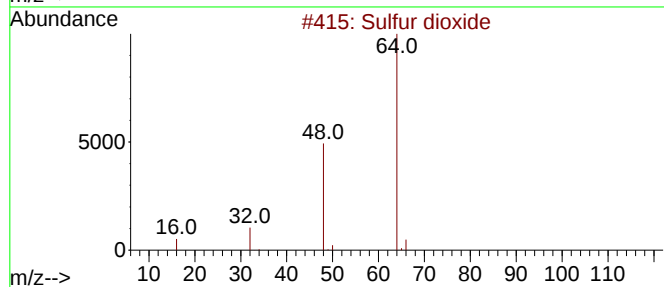
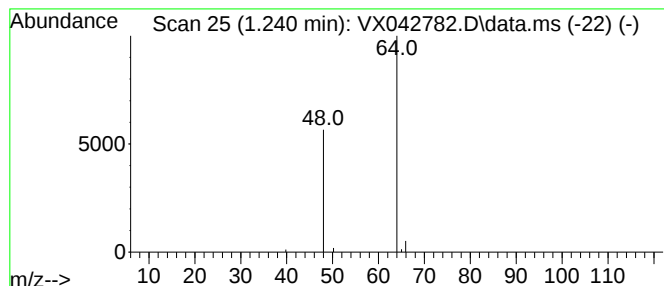
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	3.30 ug/L	19779	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	3.3	ug/L	19779	1	6.763	299399	50.0