

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122421\  
 Data File : VX026011.D  
 Acq On : 24 Dec 2021 13:30  
 Operator : JC/MD  
 Sample : M5126-06  
 Misc : 5.00mL/MSVOA\_X/WATER  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 C0J23

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs : 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122321WMA.M  
 Title : VOC Analysis

Signal : TIC: VX026011.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	54	rVB	141374	139508	13.50%	1.773%
2	1.666	91	95	104	rVB	100747	129408	12.53%	1.645%
3	2.306	194	200	209	rBV	218168	362708	35.11%	4.611%
4	2.526	232	236	245	rVB3	1852	4103	0.40%	0.052%
5	2.623	249	252	255	rBV2	318	336	0.03%	0.004%
6	2.788	276	279	286	rVB5	1024	1657	0.16%	0.021%
7	3.062	321	324	326	rBV2	290	257	0.02%	0.003%
8	3.099	326	330	333	rVV4	481	527	0.05%	0.007%
9	3.538	401	402	406	rVB2	209	273	0.03%	0.003%
10	3.782	440	442	446	rVB	249	346	0.03%	0.004%
11	3.843	450	452	456	rVB	321	371	0.04%	0.005%
12	4.026	479	482	484	rBV	272	323	0.03%	0.004%
13	4.379	538	540	541	rBV2	255	271	0.03%	0.003%
14	4.452	543	552	567	rBV	80070	233565	22.61%	2.969%
15	4.733	596	598	601	rVB2	372	404	0.04%	0.005%
16	4.812	607	611	612	rBV2	260	389	0.04%	0.005%
17	5.056	638	651	671	rBV2	117694	406999	39.39%	5.174%
18	5.221	676	678	680	rBV	466	413	0.04%	0.005%
19	5.355	698	700	702	rBV	301	292	0.03%	0.004%
20	5.531	727	729	731	rBV2	302	341	0.03%	0.004%
21	5.562	733	734	737	rVV2	425	275	0.03%	0.003%
22	5.586	737	738	743	rVB2	243	269	0.03%	0.003%
23	5.763	764	767	770	rBV2	257	299	0.03%	0.004%
24	5.970	787	801	821	rBV2	344384	1033196	100.00%	13.134%
25	6.550	894	896	899	rVB2	261	298	0.03%	0.004%
26	6.757	920	930	944	rBV	240865	581437	56.28%	7.391%
27	6.946	959	961	965	rVB2	256	264	0.03%	0.003%
28	7.104	984	987	988	rBV	783	963	0.09%	0.012%
29	7.190	999	1001	1003	rBV2	334	334	0.03%	0.004%
30	7.306	1011	1020	1033	rBV	214782	472995	45.78%	6.013%
31	7.476	1043	1048	1051	rBV3	893	1294	0.13%	0.016%
32	7.537	1055	1058	1060	rBV2	241	265	0.03%	0.003%
33	7.580	1060	1065	1072	rBV4	3093	6475	0.63%	0.082%
34	7.854	1104	1110	1119	rVB4	3410	6618	0.64%	0.084%
35	8.324	1180	1187	1200	rBV	145467	229511	22.21%	2.918%
36	8.470	1209	1211	1214	rBV2	386	512	0.05%	0.007%

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 C0J23

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs : 0.2  
 Stop Thrs : 0

Filtering: 5  
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 Max Peaks: 100  
 Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122321WMA.M  
 Title : VOC Analysis

37	8.574	1223	1228	1233	rBV3	701	1141	0.11%	0.015%
38	8.647	1233	1240	1248	rVV	537508	847408	82.02%	10.772%
39	8.714	1248	1251	1263	rVB2	8331	13539	1.31%	0.172%
40	8.952	1284	1290	1302	rVV	97311	141641	13.71%	1.801%
41	9.122	1314	1318	1319	rBV2	281	357	0.03%	0.005%
42	9.287	1339	1345	1347	rBV2	2592	5232	0.51%	0.067%
43	9.384	1355	1361	1374	rVB	374072	516501	49.99%	6.566%
44	9.525	1381	1384	1390	rVB5	1227	1916	0.19%	0.024%
45	9.677	1407	1409	1413	rVB2	254	285	0.03%	0.004%
46	9.714	1413	1415	1418	rBV2	320	302	0.03%	0.004%
47	9.951	1453	1454	1458	rVB	301	314	0.03%	0.004%
48	10.055	1465	1471	1482	rBV	535497	719802	69.67%	9.150%
49	10.177	1488	1491	1492	rBV	360	346	0.03%	0.004%
50	10.238	1498	1501	1508	rVV3	1463	1830	0.18%	0.023%
51	10.305	1508	1512	1517	rVB2	1899	2577	0.25%	0.033%
52	10.506	1540	1545	1546	rBV2	216	293	0.03%	0.004%
53	10.646	1563	1568	1572	rVV4	1168	1761	0.17%	0.022%
54	10.860	1601	1603	1608	rVB2	983	891	0.09%	0.011%
55	10.963	1617	1620	1623	rVB2	633	775	0.08%	0.010%
56	11.024	1626	1630	1637	rVB3	2048	3153	0.31%	0.040%
57	11.122	1642	1646	1651	rVB2	4543	5590	0.54%	0.071%
58	11.195	1652	1658	1666	rBV	375521	489279	47.36%	6.220%
59	11.378	1686	1688	1694	rBV3	339	575	0.06%	0.007%
60	11.476	1701	1704	1712	rVB2	1447	2517	0.24%	0.032%
61	11.628	1724	1729	1733	rBV4	516	1042	0.10%	0.013%
62	11.683	1734	1738	1740	rVV3	430	462	0.04%	0.006%
63	11.707	1740	1742	1745	rVV3	567	432	0.04%	0.005%
64	11.750	1745	1749	1754	rVB3	4529	6035	0.58%	0.077%
65	11.841	1761	1764	1769	rVB2	758	1001	0.10%	0.013%
66	11.884	1769	1771	1774	rVB2	339	338	0.03%	0.004%
67	11.933	1774	1779	1784	rBV2	2330	3425	0.33%	0.044%
68	11.975	1784	1786	1788	rVB2	472	373	0.04%	0.005%
69	12.024	1788	1794	1801	rBV	584148	719989	69.69%	9.153%
70	12.219	1819	1826	1830	rBV	3176	4792	0.46%	0.061%
71	12.323	1836	1843	1850	rBV	565066	727137	70.38%	9.243%
72	12.427	1857	1860	1864	rVB4	1333	1729	0.17%	0.022%
73	12.475	1865	1868	1869	rBV3	540	576	0.06%	0.007%
74	12.591	1884	1887	1890	rBV3	454	664	0.06%	0.008%
75	12.658	1896	1898	1902	rVB4	748	772	0.07%	0.010%
76	12.695	1902	1904	1906	rVB2	459	380	0.04%	0.005%

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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

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 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML122321WMA.M  
 Title : VOC Analysis

77	12.762	1911	1915	1921	rBV4	1005	1397	0.14%	0.018%
78	12.817	1921	1924	1927	rVB3	531	750	0.07%	0.010%
79	12.859	1927	1931	1932	rBV3	440	502	0.05%	0.006%
80	12.957	1944	1947	1948	rBV2	371	360	0.03%	0.005%
81	13.006	1953	1955	1959	rVB3	230	262	0.03%	0.003%
82	13.054	1959	1963	1967	rVB4	1061	1673	0.16%	0.021%
83	13.280	1997	2000	2002	rVV3	344	296	0.03%	0.004%
84	13.420	2020	2023	2026	rBV	333	439	0.04%	0.006%
85	13.591	2048	2051	2054	rVB3	595	755	0.07%	0.010%
86	13.695	2066	2068	2072	rVB	356	465	0.05%	0.006%
87	13.731	2072	2074	2078	rBV	245	322	0.03%	0.004%
88	13.780	2078	2082	2086	rVV2	2144	2422	0.23%	0.031%
89	13.963	2109	2112	2116	rVB3	672	873	0.08%	0.011%
90	14.006	2117	2119	2124	rVB3	390	597	0.06%	0.008%
91	14.048	2124	2126	2128	rBV	332	365	0.04%	0.005%
92	14.134	2136	2140	2145	rVB	3541	4191	0.41%	0.053%
93	14.323	2169	2171	2173	rBV2	434	351	0.03%	0.004%
94	14.396	2178	2183	2184	rBV4	507	901	0.09%	0.011%
95	14.530	2203	2205	2206	rBV	410	279	0.03%	0.004%
96	15.249	2320	2323	2325	rBV	783	571	0.06%	0.007%
97	15.396	2341	2347	2351	rBV2	1340	2795	0.27%	0.036%
98	15.609	2380	2382	2384	rBV	556	386	0.04%	0.005%
99	15.767	2406	2408	2409	rBV2	442	383	0.04%	0.005%
100	16.712	2561	2563	2566	rBV3	491	501	0.05%	0.006%

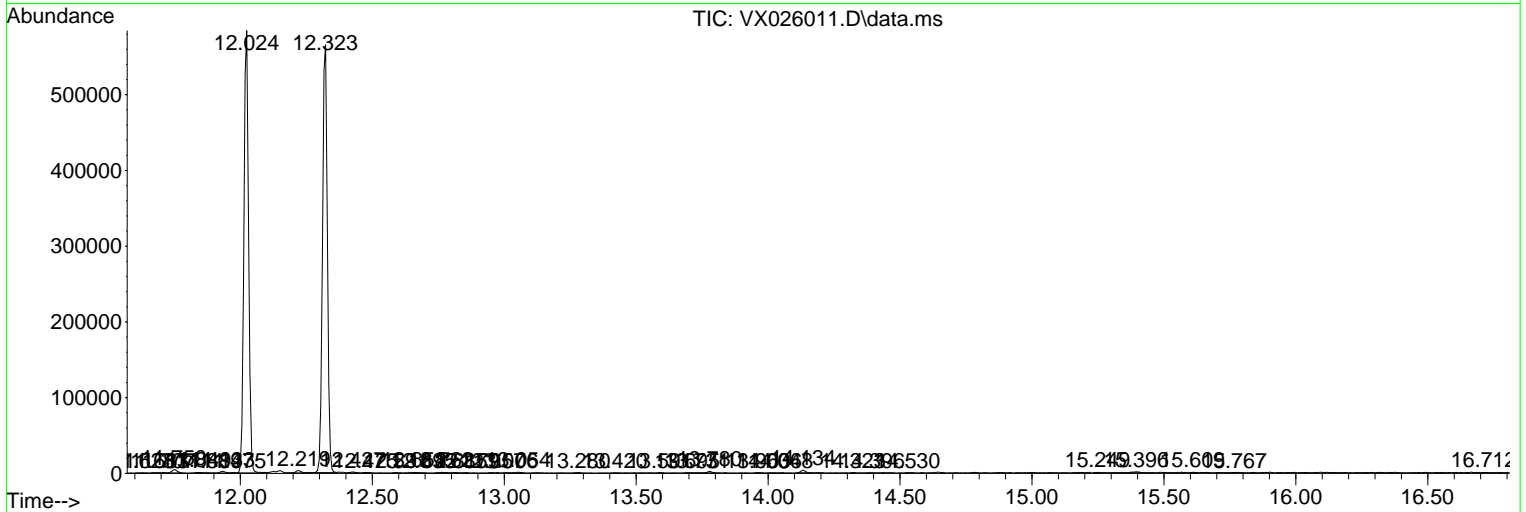
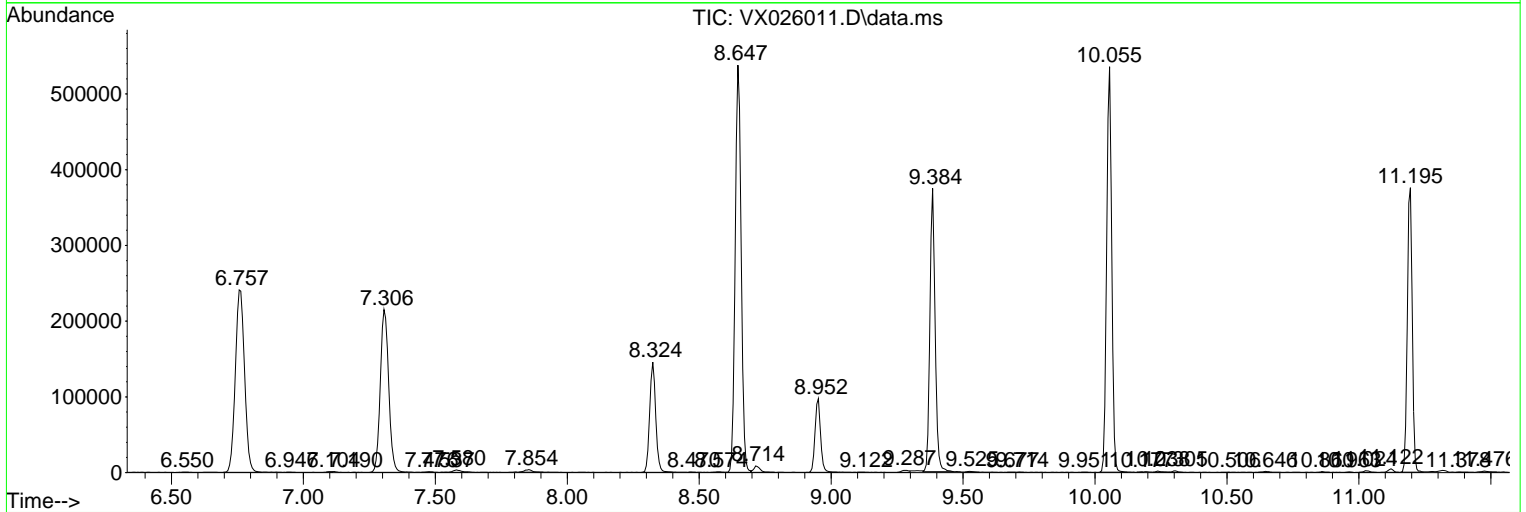
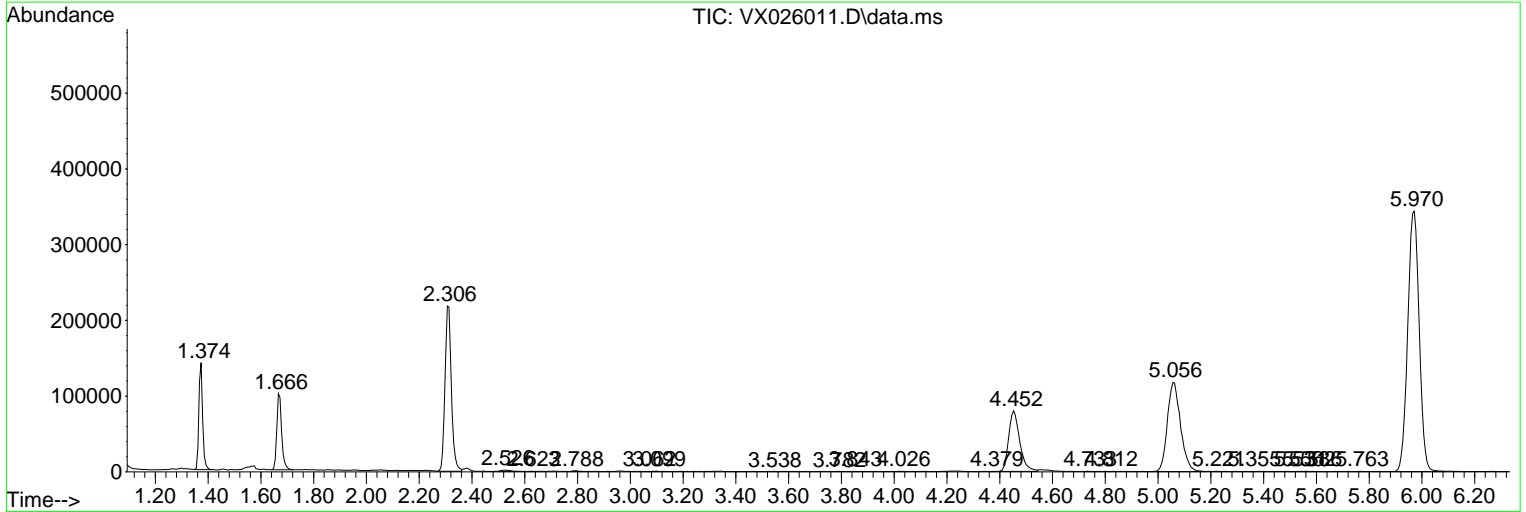
Sum of corrected areas: 7866504

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122321WMA.M  
 Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122421\  
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C0J23

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML122321WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122321WMA.M  
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc

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