

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122421\
 Data File : VX026027.D
 Acq On : 24 Dec 2021 20:02
 Operator : JC/MD
 Sample : M5150-23MS
 Misc : 5.00mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBBY0MS

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: VX026027.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.373	43	47	57	rVB2	173478	171461	0.70%	0.506%
2	1.666	91	95	104	rBV	89038	115927	0.48%	0.342%
3	2.312	194	201	209	rBV3	215173	391108	1.61%	1.154%
4	2.379	209	212	222	rVV	10282	17029	0.07%	0.050%
5	2.623	248	252	254	rBV3	311	366	0.00%	0.001%
6	2.715	262	267	270	rVB	501	824	0.00%	0.002%
7	2.763	273	275	276	rBV	319	294	0.00%	0.001%
8	2.782	276	278	279	rBV	557	417	0.00%	0.001%
9	2.965	303	308	315	rVB4	1631	3366	0.01%	0.010%
10	3.099	323	330	340	rVB2	16442	32708	0.13%	0.096%
11	3.245	349	354	356	rBV2	228	385	0.00%	0.001%
12	3.666	422	423	427	rVB2	232	251	0.00%	0.001%
13	3.721	429	432	436	rBV2	208	346	0.00%	0.001%
14	4.245	516	518	521	rVB	221	230	0.00%	0.001%
15	4.282	521	524	526	rBV2	296	354	0.00%	0.001%
16	4.318	528	530	536	rVB	318	346	0.00%	0.001%
17	4.495	544	559	585	rBV2	918556	2596717	10.66%	7.661%
18	4.934	627	631	633	rBV2	286	419	0.00%	0.001%
19	5.062	640	652	670	rVV	108789	358912	1.47%	1.059%
20	5.220	676	678	680	rBV2	267	239	0.00%	0.001%
21	5.476	712	720	730	rVB5	2479	7201	0.03%	0.021%
22	5.550	730	732	733	rVV	306	234	0.00%	0.001%
23	5.592	737	739	743	rBV2	233	272	0.00%	0.001%
24	5.647	743	748	751	rVB2	170	280	0.00%	0.001%
25	5.860	782	783	787	rVB	302	275	0.00%	0.001%
26	5.976	789	802	823	rBV2	301895	913818	3.75%	2.696%
27	6.141	828	829	833	rVB2	373	295	0.00%	0.001%
28	6.482	882	885	889	rBV2	216	300	0.00%	0.001%
29	6.549	893	896	897	rVV2	302	295	0.00%	0.001%
30	6.769	920	932	943	rBV	208751	508266	2.09%	1.500%
31	6.958	961	963	965	rBV2	244	286	0.00%	0.001%
32	7.135	980	992	1013	rVV	11572423	24359464	100.00%	71.867%
33	7.311	1014	1021	1039	rVB	189633	421314	1.73%	1.243%
34	7.580	1063	1065	1068	rVB3	358	362	0.00%	0.001%
35	7.689	1081	1083	1088	rVB2	296	289	0.00%	0.001%
36	7.878	1112	1114	1115	rBV2	396	269	0.00%	0.001%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122321WMA.M
 Title : VOC Analysis

37	7.903	1115	1118	1122	rVV3	658	1235	0.01%	0.004%
38	8.098	1148	1150	1153	rBV	237	236	0.00%	0.001%
39	8.330	1181	1188	1196	rBV	117375	195305	0.80%	0.576%
40	8.445	1205	1207	1210	rBV2	325	339	0.00%	0.001%
41	8.573	1226	1228	1234	rVB3	676	833	0.00%	0.002%
42	8.653	1234	1241	1249	rBV	476132	738661	3.03%	2.179%
43	8.726	1249	1253	1258	rVB2	7069	11307	0.05%	0.033%
44	8.842	1270	1272	1273	rVB2	465	279	0.00%	0.001%
45	8.951	1284	1290	1298	rBV	83279	120727	0.50%	0.356%
46	9.159	1319	1324	1329	rVB2	4372	6611	0.03%	0.020%
47	9.274	1338	1343	1350	rBV3	20249	33953	0.14%	0.100%
48	9.384	1356	1361	1374	rVB	346961	494310	2.03%	1.458%
49	9.634	1400	1402	1404	rVB	497	327	0.00%	0.001%
50	10.055	1465	1471	1484	rVB	480521	633957	2.60%	1.870%
51	10.195	1490	1494	1499	rVB4	781	1448	0.01%	0.004%
52	10.305	1507	1512	1517	rVV3	1486	2250	0.01%	0.007%
53	10.750	1584	1585	1590	rVB2	256	274	0.00%	0.001%
54	10.786	1590	1591	1594	rBV2	240	232	0.00%	0.001%
55	10.847	1597	1601	1606	rBV3	169	296	0.00%	0.001%
56	10.963	1617	1620	1623	rVB3	423	488	0.00%	0.001%
57	11.042	1628	1633	1635	rBV3	900	1131	0.00%	0.003%
58	11.122	1642	1646	1649	rBV2	2758	3317	0.01%	0.010%
59	11.195	1652	1658	1668	rBV	355586	444652	1.83%	1.312%
60	11.317	1674	1678	1683	rVB2	4033	6483	0.03%	0.019%
61	11.475	1702	1704	1708	rVB3	882	1096	0.00%	0.003%
62	11.542	1713	1715	1720	rBV3	333	497	0.00%	0.001%
63	11.603	1723	1725	1728	rBV	271	368	0.00%	0.001%
64	11.677	1734	1737	1738	rBV	296	309	0.00%	0.001%
65	11.750	1745	1749	1755	rVB4	3059	3755	0.02%	0.011%
66	11.847	1761	1765	1768	rVB3	535	763	0.00%	0.002%
67	11.884	1768	1771	1774	rVB	317	470	0.00%	0.001%
68	11.933	1776	1779	1783	rBV3	1283	1710	0.01%	0.005%
69	11.975	1784	1786	1788	rBV3	253	250	0.00%	0.001%
70	12.024	1788	1794	1804	rBV	505897	622011	2.55%	1.835%
71	12.128	1807	1811	1812	rBV3	1410	1571	0.01%	0.005%
72	12.225	1824	1827	1829	rBV2	456	466	0.00%	0.001%
73	12.323	1837	1843	1851	rVB	523448	637686	2.62%	1.881%
74	12.426	1858	1860	1864	rVB4	957	1159	0.00%	0.003%
75	12.664	1896	1899	1903	rVB3	438	644	0.00%	0.002%
76	12.762	1912	1915	1919	rBV	2122	2523	0.01%	0.007%

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 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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77	12.908	1936	1939	1941	rBV	212	252	0.00%	0.001%
78	13.054	1959	1963	1965	rBV2	595	711	0.00%	0.002%
79	13.146	1976	1978	1981	rBV2	279	242	0.00%	0.001%
80	13.219	1987	1990	1992	rBV2	318	352	0.00%	0.001%
81	13.493	2030	2035	2037	rBV2	341	501	0.00%	0.001%
82	13.646	2058	2060	2063	rBV2	403	354	0.00%	0.001%
83	13.780	2077	2082	2088	rVB2	1182	1583	0.01%	0.005%
84	13.908	2100	2103	2105	rVB2	276	234	0.00%	0.001%
85	13.975	2112	2114	2116	rVB	329	270	0.00%	0.001%
86	14.133	2135	2140	2147	rVB2	2559	4114	0.02%	0.012%
87	14.243	2157	2158	2160	rBV2	294	231	0.00%	0.001%
88	14.316	2167	2170	2172	rBV3	265	329	0.00%	0.001%
89	14.426	2186	2188	2190	rBV2	462	408	0.00%	0.001%
90	14.444	2190	2191	2194	rVB2	307	293	0.00%	0.001%
91	14.755	2239	2242	2245	rBV4	385	441	0.00%	0.001%
92	15.066	2291	2293	2294	rBV2	413	252	0.00%	0.001%
93	15.340	2335	2338	2339	rBV3	477	522	0.00%	0.002%
94	15.401	2342	2348	2356	rVB3	1574	3030	0.01%	0.009%
95	15.548	2371	2372	2374	rVB	485	247	0.00%	0.001%
96	15.816	2414	2416	2419	rVB2	485	432	0.00%	0.001%
97	15.847	2419	2421	2423	rBV3	446	476	0.00%	0.001%
98	16.383	2507	2509	2511	rVB3	565	377	0.00%	0.001%
99	16.633	2548	2550	2552	rBV	370	350	0.00%	0.001%
100	16.657	2552	2554	2557	rBV3	446	526	0.00%	0.002%

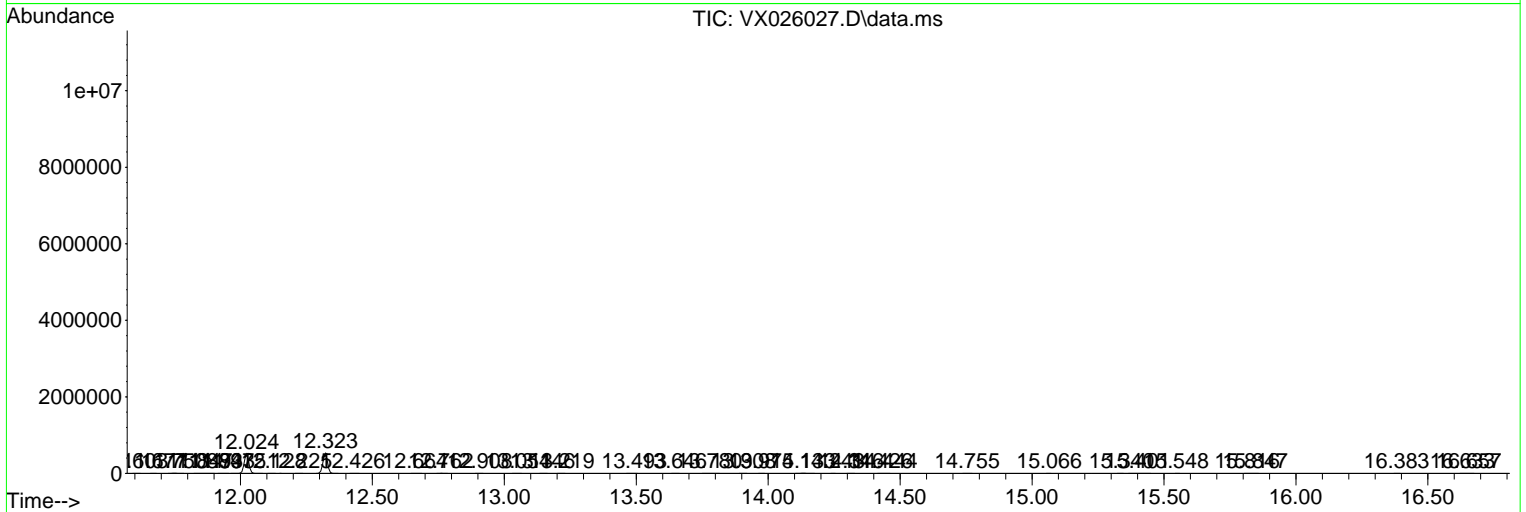
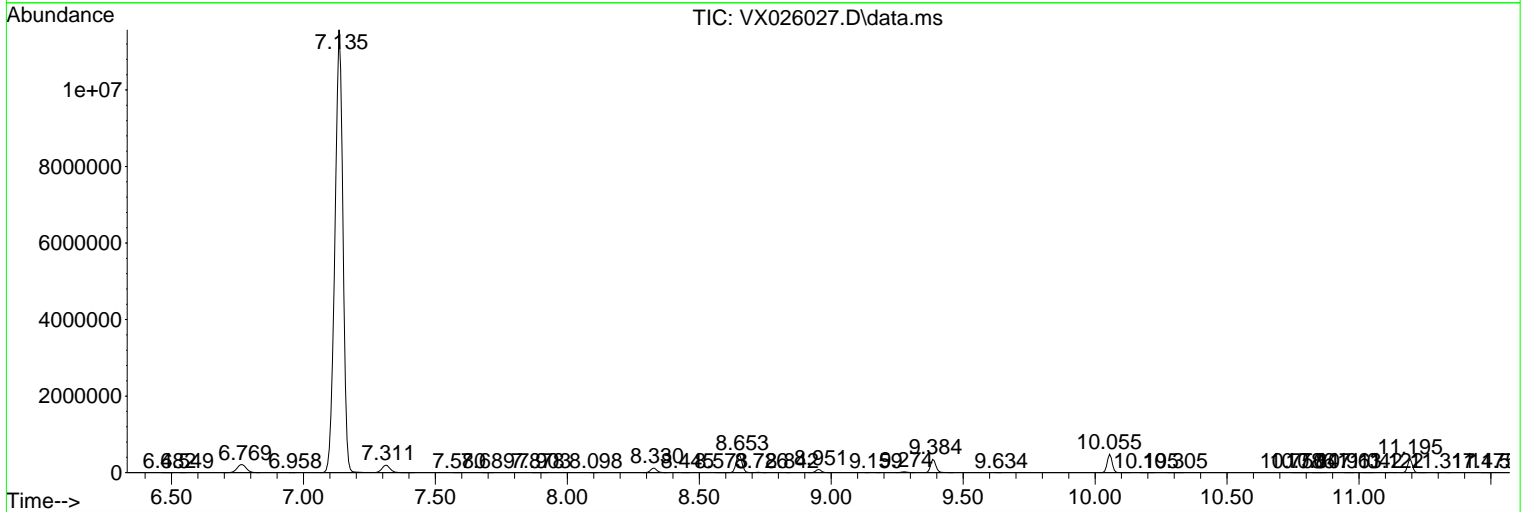
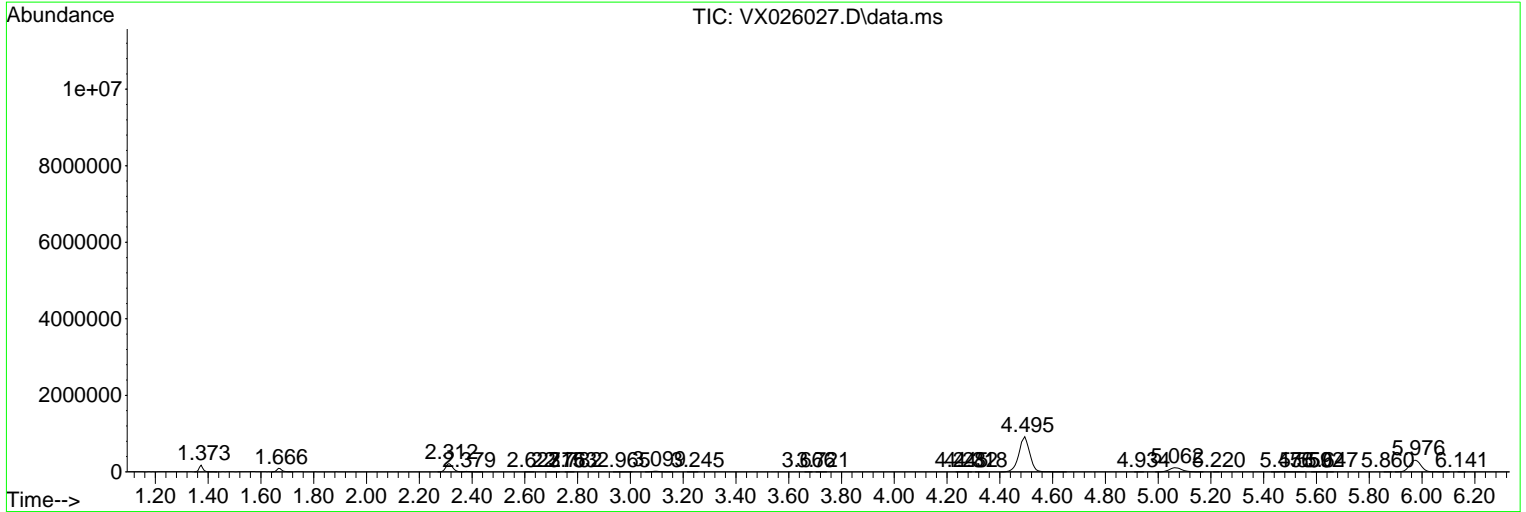
Sum of corrected areas: 33895375

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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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Instrument :
MSVOA_X
ClientSampleId :
GBBY0MS

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

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