

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122121\
 Data File : VX025965.D
 Acq On : 21 Dec 2021 18:29
 Operator : JC/MD
 Sample : M5126-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0J25

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\SFAMXML122021WMA.M
 Title : VOC Analysis

Signal : TIC: VX025965.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	33	rBV	4645	10022	1.51%	0.198%
2	1.368	43	46	54	rVB	81255	83485	12.55%	1.652%
3	1.666	91	95	105	rVB	69349	93244	14.02%	1.845%
4	2.306	193	200	209	rBV	120591	201874	30.34%	3.995%
5	2.453	223	224	229	rVB2	309	430	0.06%	0.009%
6	2.526	232	236	237	rBV2	394	517	0.08%	0.010%
7	2.611	247	250	252	rBV2	204	256	0.04%	0.005%
8	2.794	276	280	285	rVB3	478	929	0.14%	0.018%
9	2.959	297	307	314	rBV3	1192	3236	0.49%	0.064%
10	3.068	321	325	330	rVB2	255	443	0.07%	0.009%
11	3.129	332	335	338	rVB	220	243	0.04%	0.005%
12	3.331	360	368	374	rBV4	625	1415	0.21%	0.028%
13	4.160	502	504	507	rVB2	261	202	0.03%	0.004%
14	4.208	507	512	513	rBV2	485	559	0.08%	0.011%
15	4.385	538	541	543	rBV2	199	274	0.04%	0.005%
16	4.458	544	553	568	rVV	50839	144626	21.74%	2.862%
17	4.922	627	629	631	rBV2	280	212	0.03%	0.004%
18	5.056	640	651	675	rVB2	85745	268787	40.40%	5.319%
19	5.483	719	721	723	rBV2	193	221	0.03%	0.004%
20	5.550	730	732	734	rBV2	254	281	0.04%	0.006%
21	5.970	790	801	820	rVV2	214647	649305	97.60%	12.849%
22	6.476	878	884	885	rBV2	216	255	0.04%	0.005%
23	6.763	920	931	945	rBV	127264	307121	46.16%	6.078%
24	6.964	963	964	967	rBV2	324	326	0.05%	0.006%
25	7.123	983	990	999	rVB3	3107	7249	1.09%	0.143%
26	7.312	1012	1021	1037	rVV	135031	293704	44.15%	5.812%
27	7.476	1046	1048	1049	rBV	328	333	0.05%	0.007%
28	7.586	1061	1066	1073	rVV3	1500	2711	0.41%	0.054%
29	7.702	1082	1085	1088	rVB2	247	232	0.03%	0.005%
30	7.744	1088	1092	1094	rBV2	261	333	0.05%	0.007%
31	7.854	1103	1110	1117	rVB4	2193	4371	0.66%	0.086%
32	7.915	1117	1120	1121	rBV2	218	240	0.04%	0.005%
33	7.964	1127	1128	1132	rVB2	235	224	0.03%	0.004%
34	8.000	1132	1134	1137	rBV2	210	223	0.03%	0.004%
35	8.135	1153	1156	1159	rBV2	168	268	0.04%	0.005%
36	8.324	1181	1187	1195	rBV	76168	125593	18.88%	2.485%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122021WMA.M
 Title : VOC Analysis

37	8.464	1208	1210	1211	rBV	292	233	0.04%	0.005%
38	8.531	1218	1221	1223	rBV2	360	277	0.04%	0.005%
39	8.653	1233	1241	1249	rBV	422649	665296	100.00%	13.166%
40	8.720	1249	1252	1259	rVB	6492	11230	1.69%	0.222%
41	8.872	1276	1277	1280	rVB2	225	230	0.03%	0.005%
42	8.915	1280	1284	1285	rBV2	301	378	0.06%	0.007%
43	8.952	1285	1290	1302	rVV	67942	98415	14.79%	1.948%
44	9.275	1340	1343	1345	rVB2	663	562	0.08%	0.011%
45	9.384	1356	1361	1379	rBV	336184	503849	75.73%	9.971%
46	9.701	1410	1413	1414	rBV2	225	202	0.03%	0.004%
47	9.781	1425	1426	1431	rVB	270	243	0.04%	0.005%
48	9.848	1435	1437	1441	rBV2	290	269	0.04%	0.005%
49	10.055	1465	1471	1481	rBV	371579	494048	74.26%	9.777%
50	10.238	1498	1501	1506	rVV2	1014	1200	0.18%	0.024%
51	10.299	1508	1511	1518	rVB4	1035	1614	0.24%	0.032%
52	10.530	1547	1549	1554	rBV	182	260	0.04%	0.005%
53	10.634	1563	1566	1567	rBV2	387	400	0.06%	0.008%
54	10.860	1600	1603	1606	rBV3	469	599	0.09%	0.012%
55	11.037	1627	1632	1634	rVB3	516	720	0.11%	0.014%
56	11.122	1640	1646	1650	rBV4	1081	1967	0.30%	0.039%
57	11.195	1652	1658	1670	rVV	231699	307392	46.20%	6.083%
58	11.274	1670	1671	1674	rVV	242	256	0.04%	0.005%
59	11.305	1674	1676	1677	rVV	250	199	0.03%	0.004%
60	11.384	1687	1689	1690	rBV	368	277	0.04%	0.005%
61	11.475	1701	1704	1706	rVV4	543	591	0.09%	0.012%
62	11.500	1706	1708	1710	rVB2	323	285	0.04%	0.006%
63	11.677	1734	1737	1738	rVB	219	204	0.03%	0.004%
64	11.750	1746	1749	1756	rVB4	1202	1717	0.26%	0.034%
65	11.835	1761	1763	1767	rBB2	233	273	0.04%	0.005%
66	11.933	1777	1779	1782	rBV3	624	670	0.10%	0.013%
67	12.024	1789	1794	1801	rBV	272414	336037	50.51%	6.650%
68	12.091	1804	1805	1806	rBV	348	220	0.03%	0.004%
69	12.146	1812	1814	1818	rVB3	926	1178	0.18%	0.023%
70	12.219	1823	1826	1832	rVB	1866	2641	0.40%	0.052%
71	12.268	1832	1834	1836	rVB3	409	313	0.05%	0.006%
72	12.323	1836	1843	1853	rBV	315796	407502	61.25%	8.064%
73	12.433	1859	1861	1864	rVB2	444	354	0.05%	0.007%
74	12.463	1864	1866	1871	rBV2	160	220	0.03%	0.004%
75	12.634	1890	1894	1896	rVB2	168	200	0.03%	0.004%
76	13.018	1954	1957	1960	rVB2	207	239	0.04%	0.005%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.M
 Title : VOC Analysis

77	13.048	1960	1962	1964	rBV	194	234	0.04%	0.005%
78	13.176	1981	1983	1989	rBV3	215	351	0.05%	0.007%
79	13.329	2005	2008	2010	rBV	268	281	0.04%	0.006%
80	13.353	2010	2012	2015	rBV2	201	205	0.03%	0.004%
81	13.664	2061	2063	2067	rVV	193	225	0.03%	0.004%
82	14.030	2121	2123	2129	rVB2	215	305	0.05%	0.006%
83	14.134	2137	2140	2143	rVB2	205	232	0.03%	0.005%
84	14.207	2150	2152	2155	rVB2	374	290	0.04%	0.006%
85	14.420	2184	2187	2188	rVB2	193	200	0.03%	0.004%
86	14.511	2200	2202	2204	rBV2	229	238	0.04%	0.005%
87	14.847	2254	2257	2260	rBV2	328	435	0.07%	0.009%
88	15.011	2280	2284	2286	rBV2	304	430	0.06%	0.009%
89	15.085	2294	2296	2298	rBV2	250	291	0.04%	0.006%
90	15.182	2309	2312	2313	rBV2	347	300	0.05%	0.006%
91	15.274	2324	2327	2328	rBV2	200	203	0.03%	0.004%
92	15.322	2331	2335	2337	rBV2	173	240	0.04%	0.005%
93	15.444	2353	2355	2359	rBV2	258	275	0.04%	0.005%
94	15.609	2380	2382	2386	rVV2	275	300	0.05%	0.006%
95	15.658	2389	2390	2393	rBV2	202	222	0.03%	0.004%
96	15.883	2426	2427	2430	rBV2	315	355	0.05%	0.007%
97	16.231	2483	2484	2487	rBV2	292	204	0.03%	0.004%
98	16.371	2504	2507	2509	rBV	460	499	0.08%	0.010%
99	16.450	2517	2520	2521	rBV	212	238	0.04%	0.005%
100	16.737	2563	2567	2569	rBV2	240	253	0.04%	0.005%

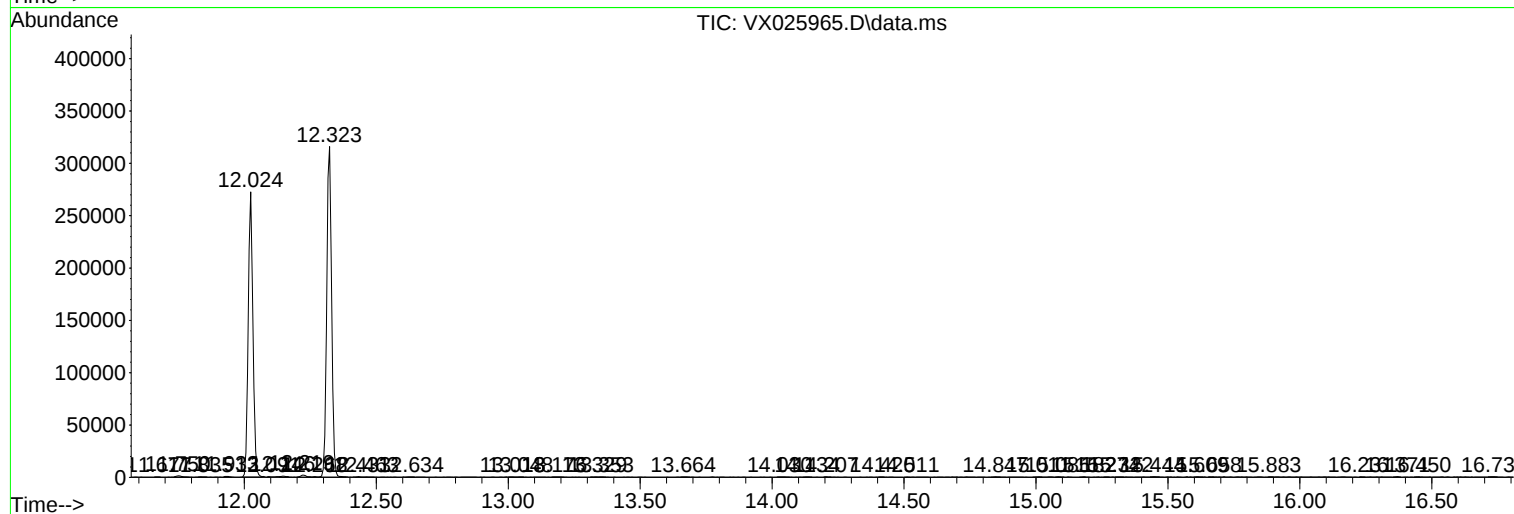
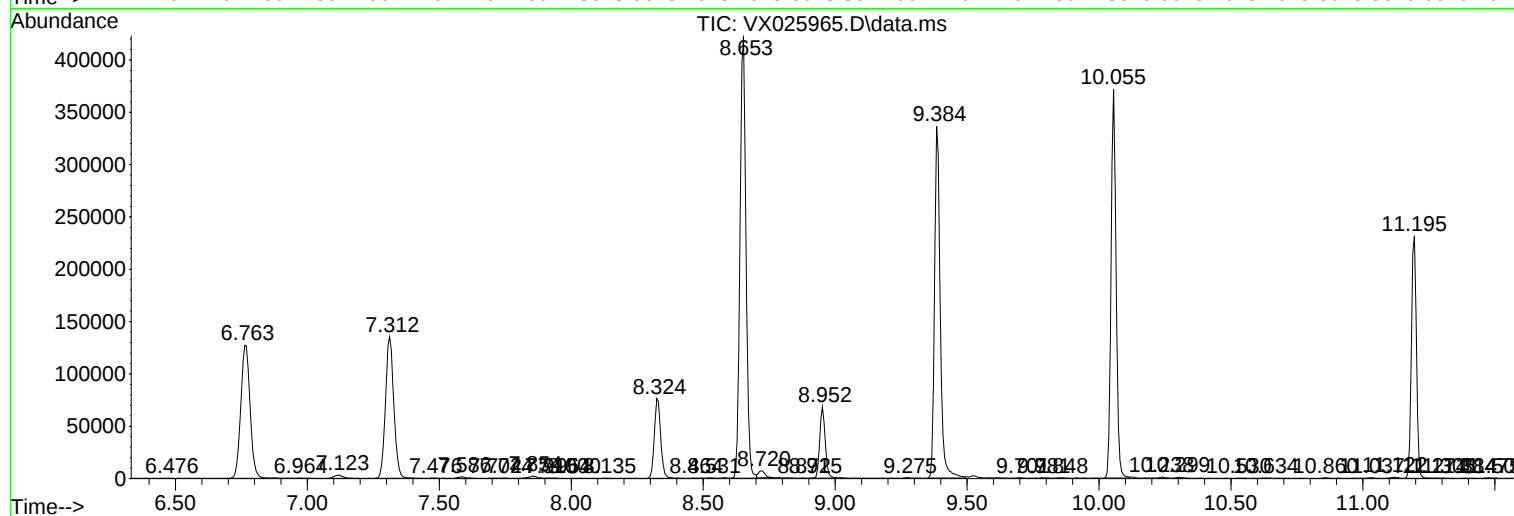
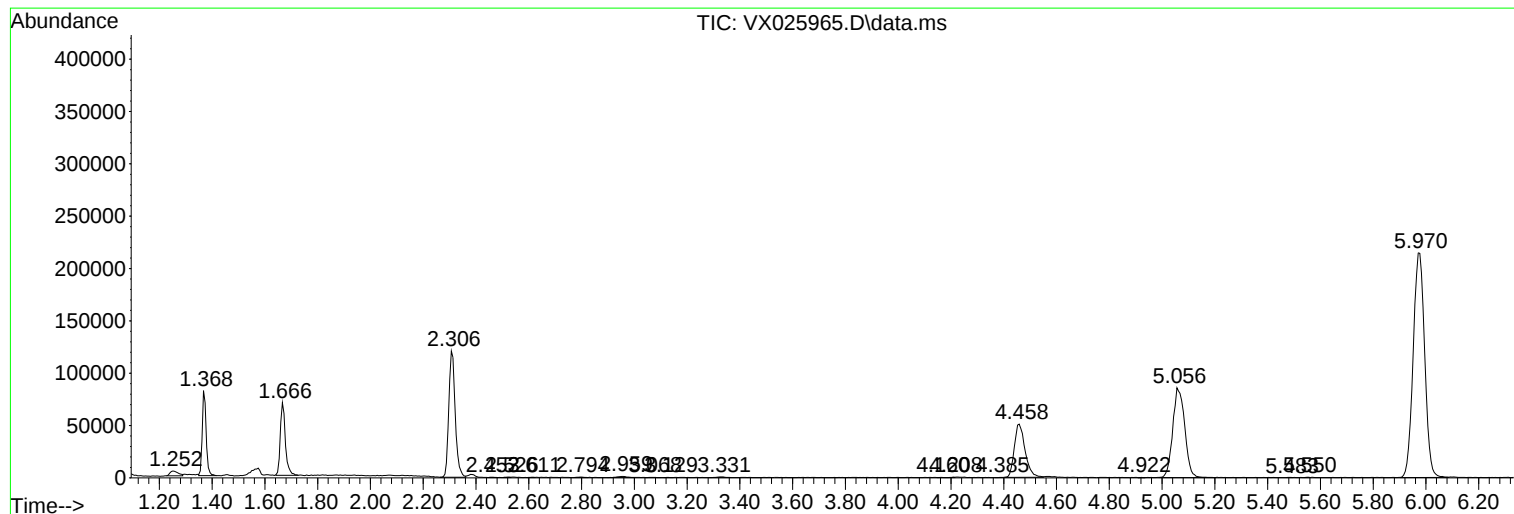
Sum of corrected areas: 5053310

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122021WMA.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\SFAMXML122021WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122121\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122021WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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