

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112621\
 Data File : VX025353.D
 Acq On : 26 Nov 2021 14:10
 Operator : JC/MD
 Sample : M4833-12
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 ESQN1

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\SFAMXML112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	24	26	32	rBV3	2173	2997	0.60%	0.075%
2	1.367	43	46	54	rVB	74155	68640	13.68%	1.726%
3	1.666	90	95	106	rVB	54488	72012	14.35%	1.811%
4	2.306	194	200	210	rBV	99480	160728	32.03%	4.042%
5	2.508	232	233	236	rBV	287	154	0.03%	0.004%
6	2.648	255	256	259	rBV2	245	216	0.04%	0.005%
7	2.794	276	280	282	rBV3	376	381	0.08%	0.010%
8	2.965	301	308	317	rVB	4442	9837	1.96%	0.247%
9	3.196	342	346	347	rBV2	160	194	0.04%	0.005%
10	3.288	358	361	364	rBV	140	200	0.04%	0.005%
11	3.428	382	384	386	rVB	141	115	0.02%	0.003%
12	3.489	392	394	397	rBV2	120	155	0.03%	0.004%
13	3.769	438	440	444	rBV2	142	196	0.04%	0.005%
14	4.062	486	488	492	rVB	129	128	0.03%	0.003%
15	4.135	499	500	503	rVV	138	106	0.02%	0.003%
16	4.184	506	508	511	rBV	109	114	0.02%	0.003%
17	4.282	521	524	526	rBV2	119	135	0.03%	0.003%
18	4.343	531	534	536	rVB2	125	139	0.03%	0.003%
19	4.452	542	552	568	rBV	43515	120272	23.96%	3.025%
20	4.592	573	575	578	rVB2	225	173	0.03%	0.004%
21	4.690	589	591	593	rVB	201	144	0.03%	0.004%
22	4.964	635	636	639	rVV	113	112	0.02%	0.003%
23	5.062	639	652	666	rVV	69770	205467	40.94%	5.167%
24	5.202	672	675	678	rBV3	164	228	0.05%	0.006%
25	5.233	678	680	683	rVV2	95	131	0.03%	0.003%
26	5.281	687	688	694	rBV2	146	285	0.06%	0.007%
27	5.330	694	696	698	rVB2	129	114	0.02%	0.003%
28	5.440	713	714	717	rBV	150	159	0.03%	0.004%
29	5.525	727	728	729	rBV	218	122	0.02%	0.003%
30	5.550	729	732	733	rBV2	215	228	0.05%	0.006%
31	5.970	789	801	816	rBV2	171289	501880	100.00%	12.622%
32	6.312	854	857	859	rBV2	108	134	0.03%	0.003%
33	6.403	870	872	875	rVV2	193	173	0.03%	0.004%
34	6.610	904	906	910	rBV2	104	140	0.03%	0.004%
35	6.763	920	931	943	rBV	139220	330172	65.79%	8.303%
36	7.110	981	988	995	rVV2	2938	6274	1.25%	0.158%

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 Title : VOC Analysis

37	7.238	1007	1009	1012	rBV2	93	106	0.02%	0.003%
38	7.312	1012	1021	1033	rVV	106727	229414	45.71%	5.769%
39	7.427	1037	1040	1041	rVB	183	129	0.03%	0.003%
40	7.482	1045	1049	1053	rBV3	285	423	0.08%	0.011%
41	7.793	1099	1100	1101	rBV	236	152	0.03%	0.004%
42	7.836	1105	1107	1110	rVB	126	112	0.02%	0.003%
43	7.927	1117	1122	1128	rBV5	796	1495	0.30%	0.038%
44	8.037	1137	1140	1143	rVB2	132	197	0.04%	0.005%
45	8.080	1145	1147	1150	rVB2	131	137	0.03%	0.003%
46	8.110	1150	1152	1154	rBV2	135	133	0.03%	0.003%
47	8.324	1181	1187	1197	rVV	73596	120511	24.01%	3.031%
48	8.470	1207	1211	1216	rVB4	514	839	0.17%	0.021%
49	8.653	1234	1241	1249	rBV	254189	404803	80.66%	10.180%
50	8.720	1249	1252	1258	rVB	3510	5432	1.08%	0.137%
51	8.903	1280	1282	1284	rBV	112	128	0.03%	0.003%
52	8.951	1284	1290	1301	rVV	56446	78195	15.58%	1.967%
53	9.092	1309	1313	1314	rBV	173	154	0.03%	0.004%
54	9.275	1339	1343	1348	rBV3	294	588	0.12%	0.015%
55	9.384	1356	1361	1380	rVB	187810	267114	53.22%	6.718%
56	9.555	1387	1389	1390	rVB	188	108	0.02%	0.003%
57	9.579	1390	1393	1394	rBV2	106	116	0.02%	0.003%
58	9.653	1402	1405	1409	rVB2	124	148	0.03%	0.004%
59	10.055	1465	1471	1489	rVB	297414	387832	77.28%	9.754%
60	10.195	1492	1494	1497	rBV	178	154	0.03%	0.004%
61	10.305	1509	1512	1517	rVB2	447	570	0.11%	0.014%
62	10.640	1565	1567	1572	rVB2	279	455	0.09%	0.011%
63	10.689	1572	1575	1576	rVB2	130	124	0.02%	0.003%
64	10.902	1608	1610	1613	rBV2	116	139	0.03%	0.003%
65	11.122	1642	1646	1649	rBV3	634	831	0.17%	0.021%
66	11.195	1652	1658	1664	rBV	205791	261888	52.18%	6.586%
67	11.311	1674	1677	1681	rBV3	385	483	0.10%	0.012%
68	11.378	1685	1688	1690	rBV2	122	171	0.03%	0.004%
69	11.695	1737	1740	1741	rBV	144	151	0.03%	0.004%
70	11.756	1746	1750	1753	rVV4	689	1116	0.22%	0.028%
71	11.933	1777	1779	1784	rVB3	370	358	0.07%	0.009%
72	12.024	1789	1794	1803	rVV	289893	362467	72.22%	9.116%
73	12.109	1806	1808	1809	rVV	151	121	0.02%	0.003%
74	12.122	1809	1810	1812	rVV2	347	288	0.06%	0.007%
75	12.152	1812	1815	1818	rVB3	648	829	0.17%	0.021%
76	12.189	1818	1821	1823	rBV2	120	119	0.02%	0.003%

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77	12.262	1830	1833	1837	rVB2	110	143	0.03%	0.004%
78	12.323	1837	1843	1850	rBV	282195	361420	72.01%	9.089%
79	12.426	1859	1860	1866	rVB2	160	143	0.03%	0.004%
80	12.469	1866	1867	1869	rBV	164	117	0.02%	0.003%
81	12.591	1885	1887	1891	rBV2	131	228	0.05%	0.006%
82	12.628	1891	1893	1896	rVB	135	123	0.02%	0.003%
83	12.756	1912	1914	1918	rVV3	154	172	0.03%	0.004%
84	13.304	1999	2004	2006	rVB2	91	143	0.03%	0.004%
85	13.378	2014	2016	2019	rBV	233	179	0.04%	0.005%
86	13.463	2027	2030	2031	rBV	118	109	0.02%	0.003%
87	13.877	2096	2098	2101	rBV	123	116	0.02%	0.003%
88	14.133	2136	2140	2143	rBV2	262	418	0.08%	0.011%
89	14.396	2181	2183	2187	rVB	168	201	0.04%	0.005%
90	14.560	2208	2210	2213	rBV	145	152	0.03%	0.004%
91	14.597	2213	2216	2219	rBV2	149	232	0.05%	0.006%
92	14.658	2224	2226	2228	rBV	194	145	0.03%	0.004%
93	14.774	2243	2245	2247	rBV	168	134	0.03%	0.003%
94	14.816	2250	2252	2253	rBV	179	112	0.02%	0.003%
95	15.176	2309	2311	2313	rVB	251	116	0.02%	0.003%
96	15.627	2383	2385	2387	rBV	195	198	0.04%	0.005%
97	15.688	2393	2395	2398	rVB3	242	165	0.03%	0.004%
98	16.560	2535	2538	2539	rBV2	175	129	0.03%	0.003%
99	16.609	2544	2546	2549	rVV3	186	130	0.03%	0.003%
100	16.767	2570	2572	2575	rBV3	179	116	0.02%	0.003%

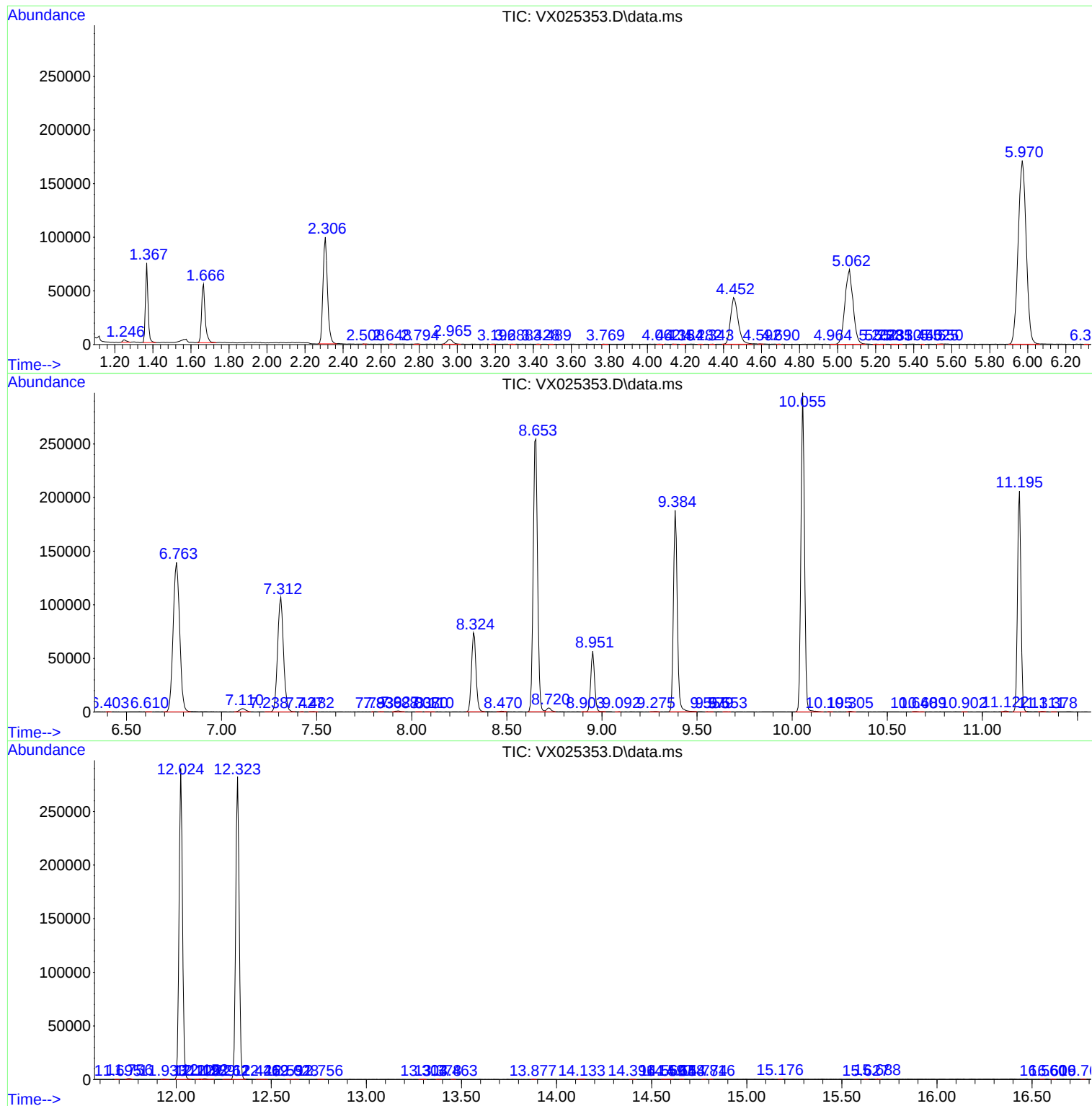
Sum of corrected areas: 3976326

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.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\SFAMXML112221WMA.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 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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