

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025653.D
 Acq On : 09 Dec 2021 11:35
 Operator : JC/MD
 Sample : VX1209MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK647

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	55	rVB	75917	77229	14.70%	1.917%
2	1.666	91	95	105	rBV	57800	77066	14.67%	1.913%
3	2.306	194	200	211	rBV	118013	192339	36.62%	4.773%
4	2.416	217	218	221	rBV	395	372	0.07%	0.009%
5	2.569	240	243	245	rBV2	316	388	0.07%	0.010%
6	2.630	251	253	255	rVV	463	332	0.06%	0.008%
7	2.648	255	256	259	rVB2	369	305	0.06%	0.008%
8	2.684	259	262	263	rBV	349	297	0.06%	0.007%
9	2.715	263	267	271	rBV2	370	729	0.14%	0.018%
10	2.794	276	280	284	rVB2	735	1028	0.20%	0.026%
11	2.947	300	305	310	rBV4	1787	3629	0.69%	0.090%
12	3.349	370	371	373	rVB	280	178	0.03%	0.004%
13	3.404	379	380	382	rBV2	210	180	0.03%	0.004%
14	3.428	382	384	386	rVB	258	193	0.04%	0.005%
15	3.453	386	388	390	rBV	244	294	0.06%	0.007%
16	3.526	398	400	401	rVB	296	197	0.04%	0.005%
17	3.648	417	420	422	rBV2	249	365	0.07%	0.009%
18	3.684	425	426	429	rBV	189	229	0.04%	0.006%
19	3.849	452	453	456	rBV	353	339	0.06%	0.008%
20	3.885	456	459	461	rBV	359	380	0.07%	0.009%
21	4.020	479	481	483	rBV	282	283	0.05%	0.007%
22	4.056	485	487	489	rBV	183	184	0.04%	0.005%
23	4.160	502	504	505	rBV	260	212	0.04%	0.005%
24	4.215	510	513	514	rBV	222	213	0.04%	0.005%
25	4.227	514	515	518	rVB	369	308	0.06%	0.008%
26	4.251	518	519	520	rBV	339	176	0.03%	0.004%
27	4.270	520	522	523	rVB	322	205	0.04%	0.005%
28	4.452	543	552	564	rBV	39013	108649	20.68%	2.696%
29	4.690	590	591	593	rBV	343	269	0.05%	0.007%
30	4.788	606	607	609	rBV	367	231	0.04%	0.006%
31	4.904	624	626	629	rBV2	216	298	0.06%	0.007%
32	5.056	638	651	664	rBV	66682	209080	39.80%	5.189%
33	5.147	664	666	668	rVB	660	462	0.09%	0.011%
34	5.513	725	726	729	rBV2	263	231	0.04%	0.006%
35	5.550	731	732	735	rVB2	291	233	0.04%	0.006%
36	5.580	735	737	740	rBV	275	293	0.06%	0.007%

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 Title : VOC Analysis

37	5.739	761	763	765	rBV	245	242	0.05%	0.006%
38	5.885	785	787	788	rBV	380	291	0.06%	0.007%
39	5.970	789	801	819	rVV2	174441	525295	100.00%	13.036%
40	6.257	846	848	849	rVB2	332	238	0.05%	0.006%
41	6.556	896	897	900	rBV	361	215	0.04%	0.005%
42	6.580	900	901	904	rBV	156	170	0.03%	0.004%
43	6.763	920	931	942	rBV	134576	320306	60.98%	7.949%
44	6.867	946	948	951	rVV	295	297	0.06%	0.007%
45	7.031	973	975	976	rBV	281	285	0.05%	0.007%
46	7.111	983	988	994	rVB4	3013	6941	1.32%	0.172%
47	7.202	1000	1003	1004	rBV	325	261	0.05%	0.006%
48	7.306	1011	1020	1032	rBV	104584	232130	44.19%	5.761%
49	7.562	1061	1062	1063	rBV	349	181	0.03%	0.004%
50	7.885	1113	1115	1116	rVB	403	233	0.04%	0.006%
51	8.232	1171	1172	1174	rVB	331	213	0.04%	0.005%
52	8.324	1181	1187	1195	rBV	74248	119145	22.68%	2.957%
53	8.598	1230	1232	1233	rVB	377	210	0.04%	0.005%
54	8.647	1233	1240	1248	rBV	280847	435156	82.84%	10.799%
55	8.714	1249	1251	1259	rVB2	3896	6270	1.19%	0.156%
56	8.775	1259	1261	1264	rBV2	217	241	0.05%	0.006%
57	8.952	1284	1290	1298	rBV	52515	76603	14.58%	1.901%
58	9.275	1338	1343	1348	rVB	4811	6290	1.20%	0.156%
59	9.317	1348	1350	1353	rVB	268	211	0.04%	0.005%
60	9.384	1355	1361	1376	rBV	173982	244005	46.45%	6.055%
61	9.695	1410	1412	1416	rVB3	552	702	0.13%	0.017%
62	9.799	1427	1429	1431	rBV	398	404	0.08%	0.010%
63	9.842	1434	1436	1437	rVV	291	197	0.04%	0.005%
64	10.006	1461	1463	1465	rBV	305	200	0.04%	0.005%
65	10.055	1465	1471	1482	rBV	281885	381500	72.63%	9.467%
66	10.256	1501	1504	1507	rBV2	349	450	0.09%	0.011%
67	10.305	1509	1512	1518	rVB3	656	1151	0.22%	0.029%
68	10.451	1535	1536	1538	rBV	315	226	0.04%	0.006%
69	10.500	1541	1544	1547	rVB	221	248	0.05%	0.006%
70	10.598	1558	1560	1563	rVB2	283	199	0.04%	0.005%
71	10.744	1582	1584	1586	rVB	319	222	0.04%	0.006%
72	10.884	1606	1607	1608	rBV	398	208	0.04%	0.005%
73	10.963	1619	1620	1622	rVB	489	227	0.04%	0.006%
74	11.122	1642	1646	1650	rBV2	1209	1573	0.30%	0.039%
75	11.189	1652	1657	1667	rVV	180599	243001	46.26%	6.030%
76	11.372	1686	1687	1691	rBV2	523	614	0.12%	0.015%

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77	11.402	1691	1692	1696	rVB2	456	447	0.09%	0.011%
78	11.457	1696	1701	1703	rBV2	524	883	0.17%	0.022%
79	11.543	1713	1715	1719	rBV2	310	432	0.08%	0.011%
80	11.750	1745	1749	1753	rBV3	1393	1748	0.33%	0.043%
81	12.024	1789	1794	1803	rBV	291446	362640	69.04%	8.999%
82	12.238	1827	1829	1831	rBV2	367	286	0.05%	0.007%
83	12.323	1837	1843	1849	rBV	289609	371933	70.80%	9.230%
84	13.116	1969	1973	1974	rBV	708	573	0.11%	0.014%
85	13.231	1990	1992	1994	rBV	345	285	0.05%	0.007%
86	13.439	2022	2026	2028	rBV2	225	338	0.06%	0.008%
87	13.481	2031	2033	2035	rBV	410	312	0.06%	0.008%
88	13.591	2049	2051	2054	rBV2	645	600	0.11%	0.015%
89	13.780	2078	2082	2088	rVB2	499	820	0.16%	0.020%
90	13.963	2110	2112	2116	rVB4	751	904	0.17%	0.022%
91	14.237	2155	2157	2159	rBV	301	233	0.04%	0.006%
92	14.469	2193	2195	2199	rBV	422	616	0.12%	0.015%
93	14.499	2199	2200	2202	rVB	356	185	0.04%	0.005%
94	14.579	2212	2213	2216	rBV2	505	498	0.09%	0.012%
95	14.737	2237	2239	2241	rVB	459	293	0.06%	0.007%
96	14.762	2241	2243	2244	rBV	416	250	0.05%	0.006%
97	14.823	2250	2253	2256	rBV2	359	584	0.11%	0.014%
98	14.993	2280	2281	2284	rVB	308	211	0.04%	0.005%
99	15.499	2362	2364	2366	rBV	405	342	0.07%	0.008%
100	16.121	2464	2466	2468	rBV2	311	230	0.04%	0.006%

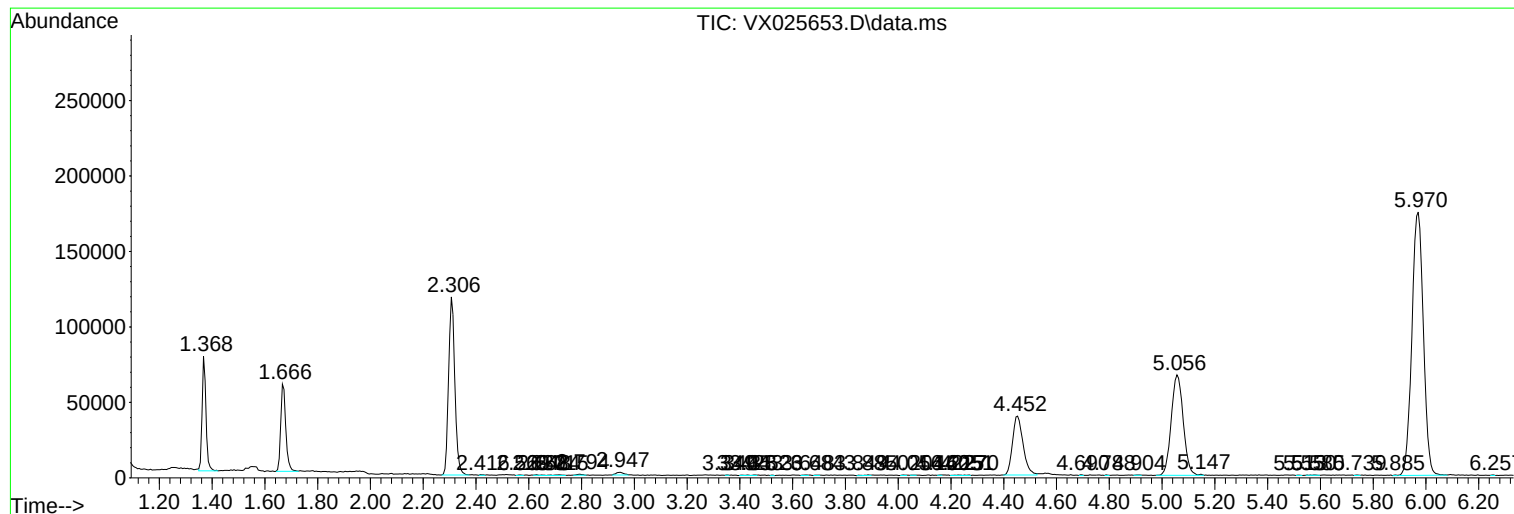
Sum of corrected areas: 4029590

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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



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TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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