

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122222\
 Data File : VX033547.D
 Acq On : 22 Dec 2022 16:11
 Operator : JC/MD
 Sample : VX1222MBL01
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK603

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\SFAMXML122222WMA.M
 Title : VOC Analysis

Signal : TIC: VX033547.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	26	29	31	rBV2	831	735	0.08%	0.011%
2	1.288	31	33	36	rVV2	448	411	0.05%	0.006%
3	1.368	42	46	58	rBV	80990	102303	11.52%	1.571%
4	1.630	85	89	91	rVV3	859	1333	0.15%	0.020%
5	1.673	91	96	109	rVB	62576	87985	9.91%	1.351%
6	1.892	129	132	135	rVB2	474	522	0.06%	0.008%
7	1.959	142	143	146	rBV2	209	214	0.02%	0.003%
8	2.136	170	172	174	rVB2	202	142	0.02%	0.002%
9	2.215	184	185	188	rVB2	286	256	0.03%	0.004%
10	2.307	194	200	210	rVB	143673	222521	25.06%	3.416%
11	2.380	210	212	214	rBV	147	166	0.02%	0.003%
12	2.514	228	234	240	rBV	1137	1921	0.22%	0.029%
13	2.624	248	252	255	rBV	119	160	0.02%	0.002%
14	2.666	257	259	260	rBV	161	141	0.02%	0.002%
15	2.715	264	267	269	rBV2	258	277	0.03%	0.004%
16	2.794	275	280	284	rBV3	1157	2197	0.25%	0.034%
17	2.825	284	285	288	rVB2	194	189	0.02%	0.003%
18	2.861	288	291	293	rBV	172	146	0.02%	0.002%
19	2.916	298	300	303	rVB	150	184	0.02%	0.003%
20	3.099	324	330	334	rBV4	588	1256	0.14%	0.019%
21	3.319	363	366	368	rBV	130	155	0.02%	0.002%
22	3.428	380	384	389	rBV2	169	360	0.04%	0.006%
23	3.538	398	402	403	rBV2	148	215	0.02%	0.003%
24	3.599	407	412	413	rBV	277	292	0.03%	0.004%
25	3.733	433	434	437	rBV2	147	149	0.02%	0.002%
26	3.819	446	448	451	rBV	195	209	0.02%	0.003%
27	3.928	465	466	470	rVB	151	153	0.02%	0.002%
28	3.965	470	472	474	rBV	168	187	0.02%	0.003%
29	4.221	510	514	516	rBV2	208	236	0.03%	0.004%
30	4.385	537	541	543	rVB2	138	151	0.02%	0.002%
31	4.453	543	552	568	rBV	53412	158775	17.88%	2.438%
32	4.642	581	583	586	rVV2	184	185	0.02%	0.003%
33	4.904	620	626	627	rBV2	294	393	0.04%	0.006%
34	5.056	638	651	670	rBV	119448	363906	40.99%	5.587%
35	5.184	670	672	673	rVB	205	139	0.02%	0.002%
36	5.257	683	684	688	rBV2	160	164	0.02%	0.003%

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 Title : VOC Analysis

37	5.367	700	702	703	rBV	283	294	0.03%	0.005%
38	5.385	703	705	707	rBV3	432	461	0.05%	0.007%
39	5.452	713	716	717	rBV2	241	227	0.03%	0.003%
40	5.556	725	733	740	rBV3	1410	3407	0.38%	0.052%
41	5.672	749	752	753	rBV2	285	373	0.04%	0.006%
42	5.867	782	784	786	rVB	193	146	0.02%	0.002%
43	5.891	786	788	789	rBV	177	147	0.02%	0.002%
44	5.964	789	800	818	rBV2	297135	887829	100.00%	13.631%
45	6.160	831	832	836	rVB2	191	185	0.02%	0.003%
46	6.208	838	840	842	rVB	229	149	0.02%	0.002%
47	6.251	845	847	851	rVB2	188	201	0.02%	0.003%
48	6.397	869	871	874	rBV	159	162	0.02%	0.002%
49	6.464	880	882	885	rBV	268	253	0.03%	0.004%
50	6.501	887	888	892	rBV	138	210	0.02%	0.003%
51	6.580	899	901	904	rBV2	119	142	0.02%	0.002%
52	6.647	909	912	914	rBV	133	181	0.02%	0.003%
53	6.757	921	930	944	rBV	222283	528526	59.53%	8.114%
54	6.909	953	955	957	rBV2	207	194	0.02%	0.003%
55	7.117	982	989	996	rBV6	1960	5020	0.57%	0.077%
56	7.306	1011	1020	1037	rBV	178019	390974	44.04%	6.003%
57	7.428	1039	1040	1043	rVB	404	336	0.04%	0.005%
58	7.470	1045	1047	1052	rBV3	320	465	0.05%	0.007%
59	7.550	1057	1060	1061	rBV2	248	259	0.03%	0.004%
60	7.830	1103	1106	1110	rBV2	410	466	0.05%	0.007%
61	7.934	1119	1123	1131	rBV2	1506	2665	0.30%	0.041%
62	8.031	1137	1139	1143	rVB2	480	516	0.06%	0.008%
63	8.062	1143	1144	1145	rBV2	286	199	0.02%	0.003%
64	8.135	1155	1156	1157	rBV	289	139	0.02%	0.002%
65	8.220	1169	1170	1174	rVB2	389	327	0.04%	0.005%
66	8.257	1174	1176	1180	rBV	241	308	0.03%	0.005%
67	8.324	1181	1187	1202	rVV	129281	206581	23.27%	3.172%
68	8.482	1208	1213	1217	rBV2	1165	2092	0.24%	0.032%
69	8.580	1225	1229	1233	rBV2	816	1152	0.13%	0.018%
70	8.647	1233	1240	1250	rBV	491345	758623	85.45%	11.647%
71	8.903	1280	1282	1284	rBV	263	210	0.02%	0.003%
72	8.952	1284	1290	1303	rVB	87305	134519	15.15%	2.065%
73	9.281	1339	1344	1346	rVB3	1188	1805	0.20%	0.028%
74	9.385	1355	1361	1378	rBV	257290	366073	41.23%	5.620%
75	9.525	1381	1384	1389	rVB3	620	1018	0.11%	0.016%
76	10.055	1465	1471	1486	rBV	421456	594190	66.93%	9.122%

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77	10.202	1490	1495	1499	rVV	1655	2212	0.25%	0.034%
78	10.305	1509	1512	1517	rVB3	1662	2294	0.26%	0.035%
79	10.647	1564	1568	1574	rBV4	1902	3732	0.42%	0.057%
80	10.714	1577	1579	1581	rBV	356	395	0.04%	0.006%
81	10.805	1591	1594	1597	rBV2	552	705	0.08%	0.011%
82	10.860	1601	1603	1608	rBV2	279	396	0.04%	0.006%
83	10.970	1617	1621	1625	rVB3	1965	2160	0.24%	0.033%
84	11.092	1640	1641	1646	rBV2	406	574	0.06%	0.009%
85	11.189	1652	1657	1664	rBV	310196	413604	46.59%	6.350%
86	11.451	1697	1700	1707	rVB4	1676	2442	0.28%	0.037%
87	11.689	1736	1739	1744	rVB4	1677	1996	0.22%	0.031%
88	11.756	1746	1750	1755	rBV3	1738	2306	0.26%	0.035%
89	11.976	1781	1786	1788	rBV2	2234	2757	0.31%	0.042%
90	12.024	1789	1794	1802	rVB	450340	568035	63.98%	8.721%
91	12.317	1837	1842	1852	rBV	494742	653420	73.60%	10.032%
92	12.890	1934	1936	1938	rBV	327	326	0.04%	0.005%
93	13.116	1969	1973	1976	rVB2	2421	2505	0.28%	0.038%
94	13.591	2047	2051	2056	rBV4	2403	3225	0.36%	0.050%
95	13.780	2078	2082	2090	rVB	3161	4217	0.47%	0.065%
96	13.963	2108	2112	2116	rVB2	3468	3790	0.43%	0.058%
97	14.439	2186	2190	2195	rBV4	817	1356	0.15%	0.021%
98	14.804	2247	2250	2251	rBV	493	489	0.06%	0.008%
99	16.408	2512	2513	2517	rVB2	710	468	0.05%	0.007%
100	16.700	2559	2561	2563	rBV	403	334	0.04%	0.005%

Sum of corrected areas: 6513490

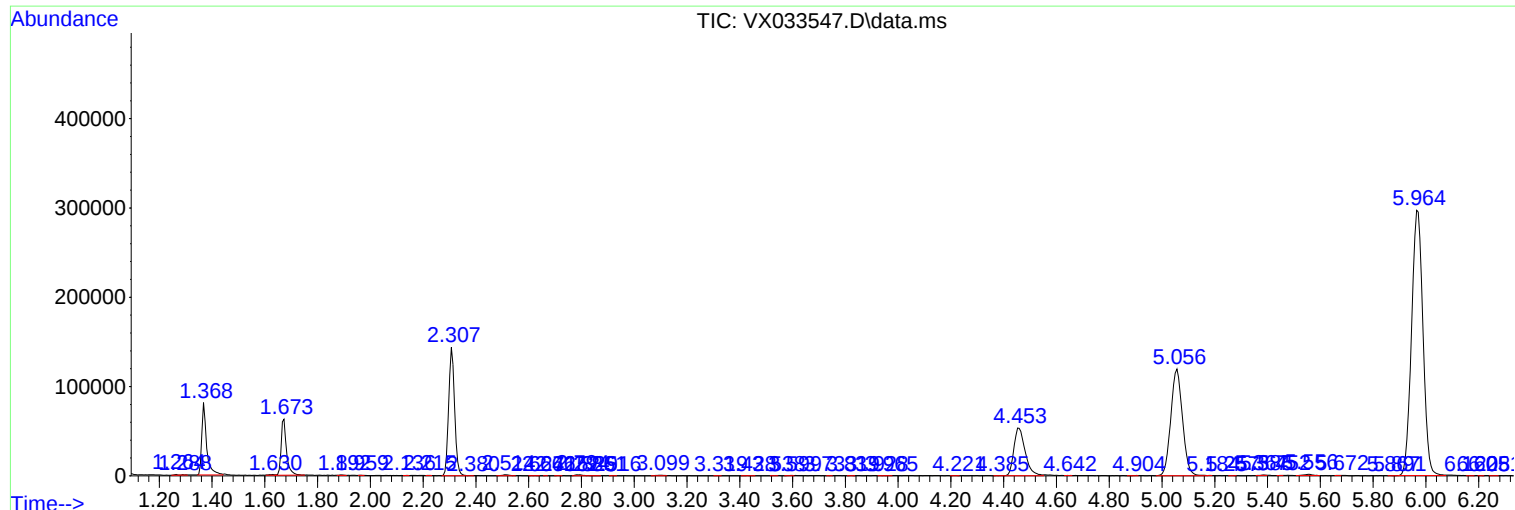
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122222WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122222WMA.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\SFAMXML122222WMA.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