

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
 Data File : VX024846.D
 Acq On : 19 Oct 2021 14:19
 Operator : JC/MD
 Sample : M4181-15ME
 Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ3ME

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\SFAMXML100721WMA.M

Title : VOC Analysis

Signal : TIC: VX024846.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	42	46	53	rBV	91441	107127	11.08%	1.307%
2	1.648	89	92	99	rBV	60424	87261	9.02%	1.065%
3	2.282	190	196	205	rVB	176086	275021	28.44%	3.356%
4	2.727	263	269	271	rBV2	2002	3449	0.36%	0.042%
5	3.355	370	372	375	rVB3	695	824	0.09%	0.010%
6	3.416	379	382	383	rBV2	828	981	0.10%	0.012%
7	3.593	408	411	413	rBV2	778	834	0.09%	0.010%
8	4.007	477	479	480	rBV	888	637	0.07%	0.008%
9	4.203	508	511	514	rVB2	487	585	0.06%	0.007%
10	4.294	518	526	535	rVB4	3398	9513	0.98%	0.116%
11	4.361	535	537	541	rVB3	515	681	0.07%	0.008%
12	4.495	547	559	584	rBV	63576	282065	29.16%	3.442%
13	5.062	639	652	673	rBV2	126026	399202	41.27%	4.871%
14	5.391	701	706	707	rBV2	808	1318	0.14%	0.016%
15	5.458	710	717	718	rBV5	4361	7966	0.82%	0.097%
16	5.599	738	740	741	rBV2	893	762	0.08%	0.009%
17	5.678	752	753	759	rVB2	655	861	0.09%	0.011%
18	5.806	771	774	776	rBV2	1118	1376	0.14%	0.017%
19	5.971	789	801	820	rBV2	339136	967182	100.00%	11.801%
20	6.251	843	847	853	rVB5	1521	3295	0.34%	0.040%
21	6.355	855	864	865	rBV5	5362	10497	1.09%	0.128%
22	6.598	900	904	907	rBV4	1493	1991	0.21%	0.024%
23	6.763	921	931	943	rBV	288581	689014	71.24%	8.407%
24	6.970	963	965	969	rVB	581	631	0.07%	0.008%
25	7.111	981	988	999	rBV6	7221	18327	1.89%	0.224%
26	7.220	999	1006	1011	rBV4	3022	7779	0.80%	0.095%
27	7.312	1013	1021	1028	rBV	206227	454269	46.97%	5.543%
28	7.470	1045	1047	1049	rBV2	1222	1220	0.13%	0.015%
29	7.775	1091	1097	1102	rVV4	2613	5806	0.60%	0.071%
30	7.812	1102	1103	1106	rVB	962	615	0.06%	0.008%
31	7.915	1115	1120	1121	rVV4	582	981	0.10%	0.012%
32	7.958	1121	1127	1135	rVB8	4190	10239	1.06%	0.125%
33	8.049	1141	1142	1147	rBV3	693	847	0.09%	0.010%
34	8.226	1168	1171	1174	rBV3	900	1299	0.13%	0.016%
35	8.275	1176	1179	1181	rVV4	2367	3281	0.34%	0.040%
36	8.330	1181	1188	1200	rVB	136640	228661	23.64%	2.790%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML100721WMA.M
 Title : VOC Analysis

37	8.519	1217	1219	1220	rVB2	1135	638	0.07%	0.008%
38	8.604	1226	1233	1234	rBV5	4248	7811	0.81%	0.095%
39	8.653	1235	1241	1248	rVB	470849	745475	77.08%	9.096%
40	8.720	1248	1252	1255	rBV2	10239	14189	1.47%	0.173%
41	8.909	1277	1283	1285	rBV4	2256	3245	0.34%	0.040%
42	8.952	1285	1290	1300	rVB	100221	160907	16.64%	1.963%
43	9.104	1312	1315	1318	rBV4	1568	2011	0.21%	0.025%
44	9.281	1338	1344	1346	rBV3	971	1329	0.14%	0.016%
45	9.397	1356	1363	1378	rBV	270119	562071	58.11%	6.858%
46	9.567	1387	1391	1394	rVB3	5307	8019	0.83%	0.098%
47	9.622	1396	1400	1404	rBV3	2918	4766	0.49%	0.058%
48	9.756	1420	1422	1428	rVB5	1515	2387	0.25%	0.029%
49	9.823	1428	1433	1440	rBV6	3281	6405	0.66%	0.078%
50	9.915	1444	1448	1450	rVB2	1263	1701	0.18%	0.021%
51	9.958	1450	1455	1458	rBV3	585	869	0.09%	0.011%
52	10.006	1460	1463	1465	rBV2	1270	1567	0.16%	0.019%
53	10.055	1465	1471	1481	rBV	566368	799701	82.68%	9.757%
54	10.195	1490	1494	1498	rVB2	3236	5132	0.53%	0.063%
55	10.305	1509	1512	1517	rVB3	9721	15341	1.59%	0.187%
56	10.360	1517	1521	1528	rVB5	5419	8671	0.90%	0.106%
57	10.458	1535	1537	1541	rVB4	791	939	0.10%	0.011%
58	10.646	1564	1568	1577	rVB	12252	17062	1.76%	0.208%
59	10.756	1582	1586	1587	rBV3	2520	2999	0.31%	0.037%
60	10.860	1599	1603	1606	rBV4	3953	5458	0.56%	0.067%
61	10.896	1606	1609	1613	rVB3	3230	4317	0.45%	0.053%
62	10.964	1616	1620	1624	rBV2	4943	6490	0.67%	0.079%
63	11.037	1629	1632	1637	rVB4	1475	1725	0.18%	0.021%
64	11.085	1637	1640	1642	rBV3	1503	1653	0.17%	0.020%
65	11.195	1652	1658	1669	rBV	369317	508682	52.59%	6.207%
66	11.305	1674	1676	1680	rVB	2952	3758	0.39%	0.046%
67	11.384	1686	1689	1695	rVB4	5786	7908	0.82%	0.096%
68	11.433	1695	1697	1698	rBV2	1336	1284	0.13%	0.016%
69	11.451	1698	1700	1702	rBV3	2275	2675	0.28%	0.033%
70	11.616	1723	1727	1733	rVB2	4095	6224	0.64%	0.076%
71	11.719	1740	1744	1746	rBV3	3587	4376	0.45%	0.053%
72	11.756	1746	1750	1757	rVB2	12286	17309	1.79%	0.211%
73	11.902	1769	1774	1777	rVB3	2752	3490	0.36%	0.043%
74	11.945	1777	1781	1784	rBV5	2364	4822	0.50%	0.059%
75	12.024	1789	1794	1801	rBV	625170	807430	83.48%	9.852%
76	12.268	1832	1834	1837	rVB	1961	1992	0.21%	0.024%

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 Title : VOC Analysis

77	12.323	1837	1843	1850	rBV	580076	726410	75.11%	8.863%
78	12.427	1856	1860	1864	rBV	7716	9305	0.96%	0.114%
79	12.536	1874	1878	1880	rBV2	2339	2605	0.27%	0.032%
80	12.768	1913	1916	1918	rBV2	1445	1293	0.13%	0.016%
81	12.890	1933	1936	1939	rBV4	1601	2215	0.23%	0.027%
82	12.975	1946	1950	1955	rVB6	3053	5468	0.57%	0.067%
83	13.042	1955	1961	1962	rBV4	1179	2331	0.24%	0.028%
84	13.268	1995	1998	2001	rBV	6876	7350	0.76%	0.090%
85	13.384	2013	2017	2021	rBV4	3221	4779	0.49%	0.058%
86	13.591	2046	2051	2055	rBV6	2174	3562	0.37%	0.043%
87	13.737	2071	2075	2076	rBV3	900	1244	0.13%	0.015%
88	13.780	2078	2082	2085	rVV	15968	18409	1.90%	0.225%
89	14.036	2121	2124	2128	rBV2	5059	5873	0.61%	0.072%
90	14.103	2133	2135	2139	rVB4	1925	2589	0.27%	0.032%
91	14.170	2144	2146	2148	rVB3	1608	972	0.10%	0.012%
92	14.402	2182	2184	2187	rBV3	922	631	0.07%	0.008%
93	14.512	2198	2202	2206	rVB6	2234	3594	0.37%	0.044%
94	14.640	2220	2223	2232	rVB2	11257	14855	1.54%	0.181%
95	14.780	2239	2246	2253	rBV3	12303	21612	2.23%	0.264%
96	15.091	2295	2297	2298	rBV2	973	759	0.08%	0.009%
97	15.213	2314	2317	2321	rVB6	3067	3917	0.40%	0.048%
98	15.615	2380	2383	2386	rBV3	2793	3478	0.36%	0.042%
99	16.078	2457	2459	2460	rBV2	1122	764	0.08%	0.009%
100	16.377	2505	2508	2513	rBV5	1781	2671	0.28%	0.033%

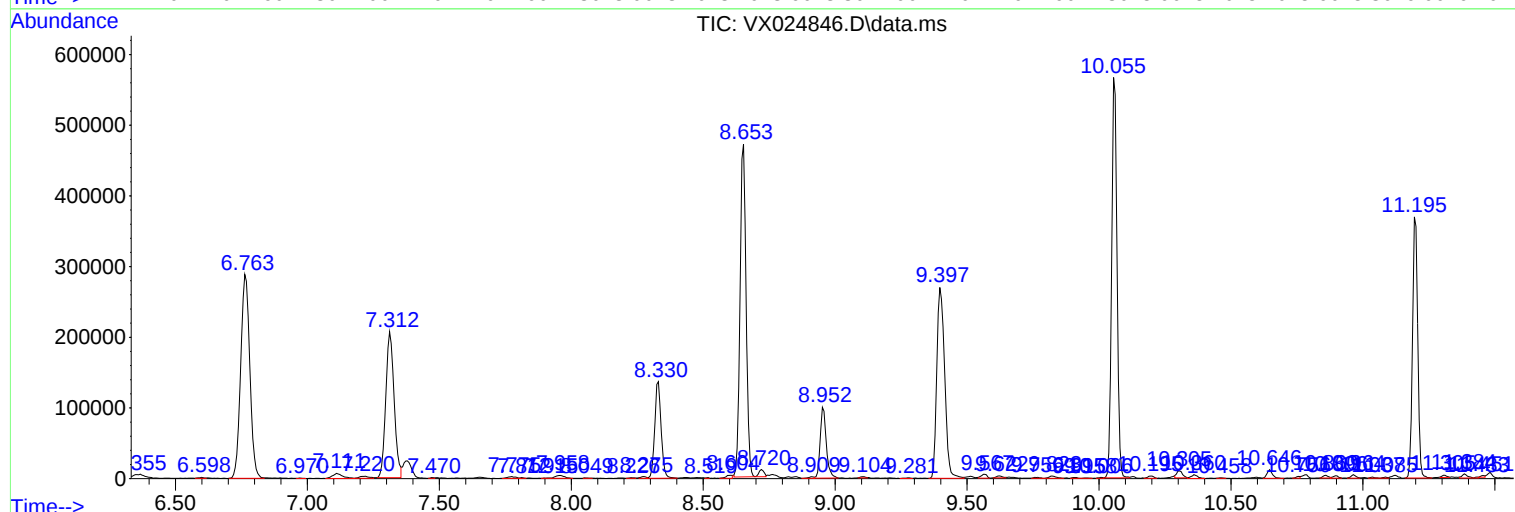
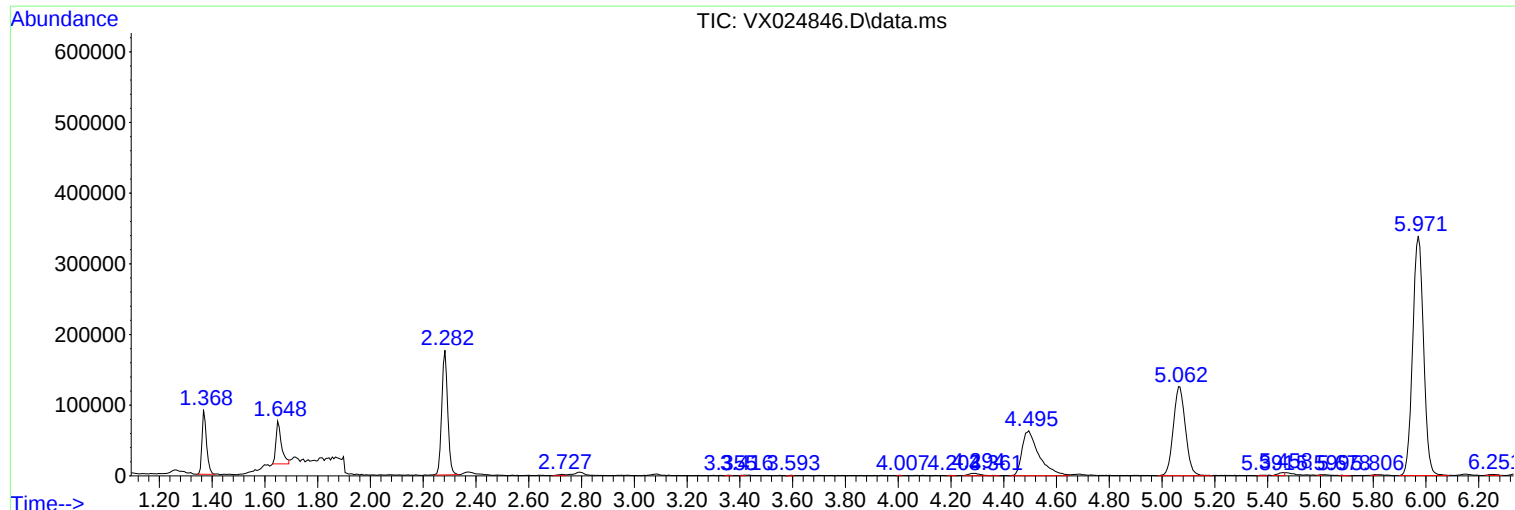
Sum of corrected areas: 8195911

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Instrument :
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ClientSampleId :
C0AZ3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM100721WMA.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\SFAMXML100721WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
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No Library Search Compounds Detected

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