

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039326.D
 Acq On : 18 Dec 2023 21:13
 Operator : JC/MD
 Sample : 05835-08 100X
 Misc : 5.27g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AQ0

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039326.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	55	rBV	91897	95490	11.15%	1.373%
2	1.666	91	95	109	rVB	63927	90279	10.54%	1.298%
3	2.307	194	200	211	rBV	169850	265863	31.05%	3.824%
4	2.477	226	228	230	rBV2	223	217	0.03%	0.003%
5	2.788	275	279	289	rVB4	1390	2811	0.33%	0.040%
6	2.947	297	305	312	rVB3	2038	4568	0.53%	0.066%
7	3.008	312	315	317	rBV2	189	219	0.03%	0.003%
8	3.245	351	354	357	rBV2	277	387	0.05%	0.006%
9	3.520	398	399	401	rVB	304	169	0.02%	0.002%
10	3.544	401	403	405	rBV2	162	169	0.02%	0.002%
11	3.636	415	418	419	rBV2	203	173	0.02%	0.002%
12	3.684	424	426	429	rVV2	169	213	0.02%	0.003%
13	3.770	438	440	444	rVB2	276	318	0.04%	0.005%
14	3.861	454	455	458	rBV2	216	198	0.02%	0.003%
15	3.892	458	460	465	rVB2	190	214	0.02%	0.003%
16	3.989	474	476	477	rBV	272	207	0.02%	0.003%
17	4.044	483	485	489	rVB2	192	254	0.03%	0.004%
18	4.251	516	519	520	rVV2	201	172	0.02%	0.002%
19	4.452	544	552	569	rBV	88403	251544	29.38%	3.618%
20	4.696	591	592	595	rBV2	323	365	0.04%	0.005%
21	4.916	626	628	631	rVB2	334	283	0.03%	0.004%
22	4.952	631	634	637	rBV2	278	291	0.03%	0.004%
23	5.056	637	651	671	rBV	112464	341222	39.85%	4.907%
24	5.483	714	721	722	rBV4	403	707	0.08%	0.010%
25	5.690	752	755	756	rBV	176	167	0.02%	0.002%
26	5.812	773	775	776	rBV	351	245	0.03%	0.004%
27	5.971	788	801	824	rBV2	277388	856186	100.00%	12.313%
28	6.306	854	856	859	rVV2	229	230	0.03%	0.003%
29	6.336	859	861	864	rVB2	262	260	0.03%	0.004%
30	6.403	867	872	875	rBV2	277	424	0.05%	0.006%
31	6.452	878	880	882	rBV2	245	253	0.03%	0.004%
32	6.519	886	891	893	rVV2	239	434	0.05%	0.006%
33	6.678	914	917	918	rBV2	150	189	0.02%	0.003%
34	6.763	922	931	952	rBV	221753	545147	63.67%	7.840%
35	6.970	963	965	967	rBV2	437	235	0.03%	0.003%
36	7.117	984	989	995	rBV3	1261	2636	0.31%	0.038%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

37	7.202	999	1003	1008	rVB2	205	325	0.04%	0.005%
38	7.306	1011	1020	1038	rBV	174592	392977	45.90%	5.652%
39	7.470	1046	1047	1049	rBV2	620	487	0.06%	0.007%
40	7.927	1120	1122	1123	rBV	246	212	0.02%	0.003%
41	8.074	1142	1146	1148	rBV2	249	328	0.04%	0.005%
42	8.238	1170	1173	1175	rBV2	259	251	0.03%	0.004%
43	8.324	1181	1187	1198	rBV	120338	198007	23.13%	2.848%
44	8.501	1214	1216	1218	rBV3	242	218	0.03%	0.003%
45	8.525	1218	1220	1222	rVB2	295	211	0.02%	0.003%
46	8.574	1225	1228	1230	rBV2	539	536	0.06%	0.008%
47	8.647	1234	1240	1257	rBV	408220	659773	77.06%	9.489%
48	8.854	1271	1274	1276	rBV2	235	232	0.03%	0.003%
49	8.952	1284	1290	1299	rBV	88678	132516	15.48%	1.906%
50	9.281	1339	1344	1348	rBV3	804	1172	0.14%	0.017%
51	9.385	1355	1361	1380	rBV	401718	579898	67.73%	8.340%
52	9.695	1410	1412	1416	rBV3	467	669	0.08%	0.010%
53	9.848	1435	1437	1439	rVB	238	177	0.02%	0.003%
54	9.897	1443	1445	1448	rVB2	179	187	0.02%	0.003%
55	10.055	1465	1471	1474	rBV	491448	787102	91.93%	11.320%
56	10.201	1491	1495	1499	rVB3	662	1023	0.12%	0.015%
57	10.256	1503	1504	1507	rBV	308	243	0.03%	0.003%
58	10.305	1507	1512	1519	rVV3	420	878	0.10%	0.013%
59	10.561	1552	1554	1555	rBV2	334	171	0.02%	0.002%
60	10.640	1565	1567	1573	rBV4	504	1026	0.12%	0.015%
61	10.878	1604	1606	1609	rVB	315	237	0.03%	0.003%
62	10.915	1609	1612	1614	rBV2	154	172	0.02%	0.002%
63	10.964	1617	1620	1624	rVV	586	685	0.08%	0.010%
64	11.092	1638	1641	1645	rVB4	569	753	0.09%	0.011%
65	11.189	1651	1657	1665	rBV	333195	436454	50.98%	6.277%
66	11.366	1683	1686	1690	rBV3	757	848	0.10%	0.012%
67	11.457	1699	1701	1702	rBV	702	499	0.06%	0.007%
68	11.811	1755	1759	1761	rBV2	174	223	0.03%	0.003%
69	11.969	1781	1785	1788	rBV	3778	4289	0.50%	0.062%
70	12.018	1788	1793	1810	rVB	503117	690038	80.59%	9.924%
71	12.317	1837	1842	1851	rBV	457743	587226	68.59%	8.445%
72	12.530	1873	1877	1879	rVB2	251	240	0.03%	0.003%
73	12.762	1911	1915	1919	rVB	725	883	0.10%	0.013%
74	12.811	1922	1923	1927	rVB	245	205	0.02%	0.003%
75	13.024	1955	1958	1961	rVB2	243	348	0.04%	0.005%
76	13.055	1961	1963	1964	rBV2	220	227	0.03%	0.003%

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Title : VOC Analysis

77	13.128	1970	1975	1978	rVB3	383	576	0.07%	0.008%
78	13.158	1978	1980	1982	rBV2	172	179	0.02%	0.003%
79	13.183	1982	1984	1986	rVV	210	215	0.03%	0.003%
80	13.335	2008	2009	2011	rBV2	214	188	0.02%	0.003%
81	13.500	2033	2036	2038	rBV2	161	220	0.03%	0.003%
82	13.591	2048	2051	2055	rVB3	681	867	0.10%	0.012%
83	13.646	2057	2060	2062	rVB2	219	187	0.02%	0.003%
84	13.780	2080	2082	2087	rVB3	538	691	0.08%	0.010%
85	13.853	2092	2094	2099	rBV2	151	175	0.02%	0.003%
86	13.975	2109	2114	2117	rVB3	456	651	0.08%	0.009%
87	14.128	2135	2139	2144	rVV2	1559	1730	0.20%	0.025%
88	14.176	2145	2147	2152	rVB2	268	370	0.04%	0.005%
89	14.317	2166	2170	2172	rVV3	142	176	0.02%	0.003%
90	14.688	2228	2231	2234	rVB2	219	276	0.03%	0.004%
91	14.774	2243	2245	2248	rVB2	245	244	0.03%	0.004%
92	14.798	2248	2249	2251	rBV2	257	169	0.02%	0.002%
93	15.322	2334	2335	2337	rVB	303	166	0.02%	0.002%
94	15.353	2337	2340	2341	rBV2	225	221	0.03%	0.003%
95	15.444	2353	2355	2356	rBV2	301	193	0.02%	0.003%
96	15.816	2413	2416	2418	rBV3	281	295	0.03%	0.004%
97	15.920	2432	2433	2434	rBV	346	176	0.02%	0.003%
98	16.475	2522	2524	2526	rVB	294	220	0.03%	0.003%
99	16.639	2549	2551	2554	rVB2	206	228	0.03%	0.003%
100	16.682	2555	2558	2559	rBV	293	272	0.03%	0.004%

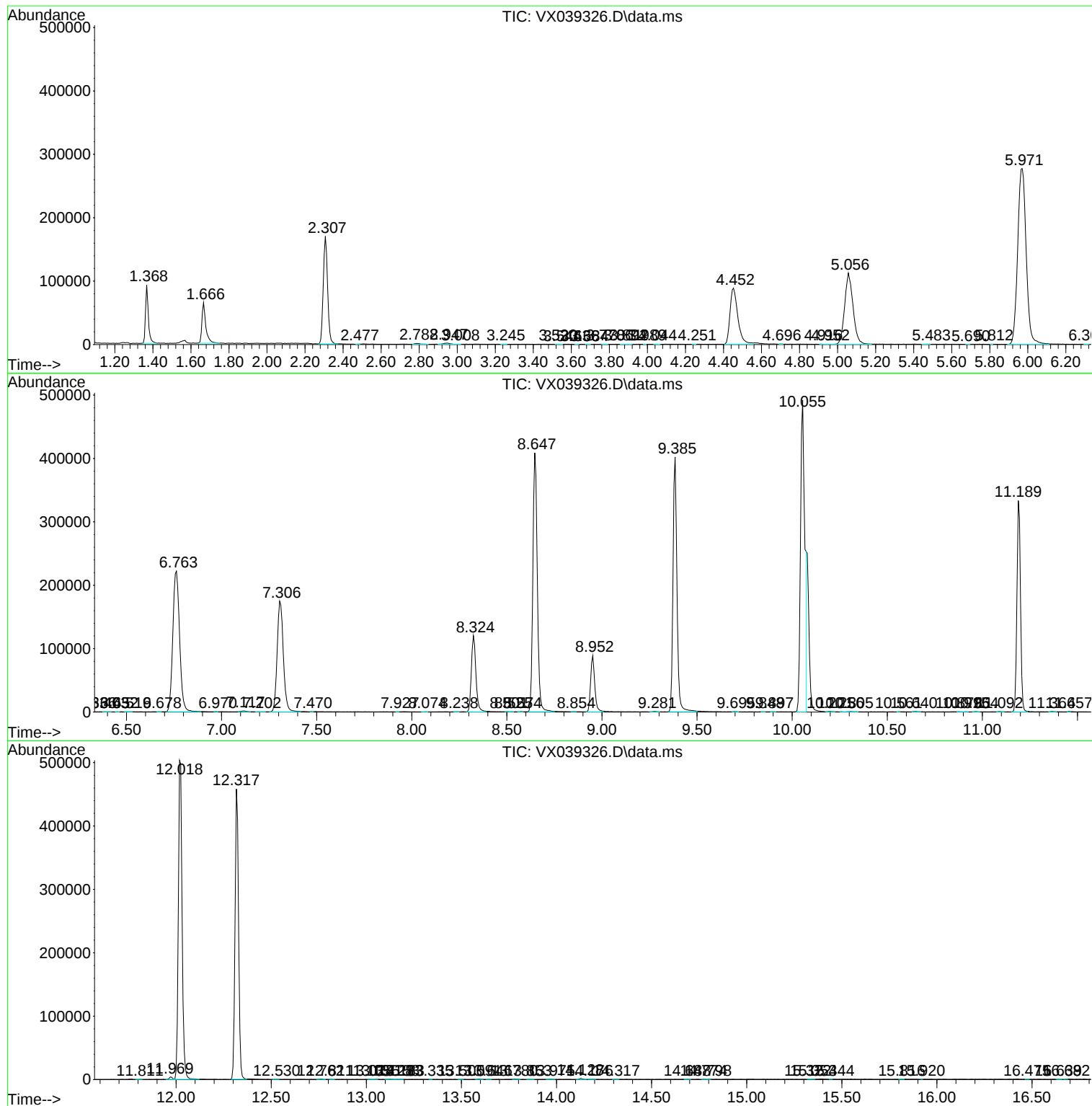
Sum of corrected areas: 6953370

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.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\SFAMXML120523WMA.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\NIST20.L
TIC Integration Parameters: LSCINT.P

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