

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX122821\  
 Data File : VX026124.D  
 Acq On : 29 Dec 2021 01:47  
 Operator : JC/MD  
 Sample : M5233-06 10X  
 Misc : 8.49g/5mL/100uL/5.00mL/MSVOA\_X/MEOH  
 ALS Vial : 31 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 GBCC4

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\SFAMXLM122821WMA.M  
 Title : VOC Analysis

Signal : TIC: VX026124.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	54	rVB	131839	139750	15.29%	2.131%
2	1.666	91	95	104	rVB	108045	123742	13.54%	1.887%
3	2.313	195	201	213	rBV	208822	344071	37.65%	5.246%
4	2.678	259	261	264	rBV2	529	655	0.07%	0.010%
5	2.794	275	280	286	rBV3	2447	4509	0.49%	0.069%
6	2.947	300	305	314	rVB3	7708	18172	1.99%	0.277%
7	3.075	324	326	329	rBV2	485	479	0.05%	0.007%
8	3.215	347	349	352	rVV	676	515	0.06%	0.008%
9	3.611	411	414	417	rBV2	646	873	0.10%	0.013%
10	3.727	431	433	435	rBV	739	573	0.06%	0.009%
11	3.855	452	454	457	rVB	671	565	0.06%	0.009%
12	4.032	479	483	485	rBV	500	641	0.07%	0.010%
13	4.294	522	526	528	rBV	530	618	0.07%	0.009%
14	4.367	536	538	543	rBV	589	536	0.06%	0.008%
15	4.465	545	554	569	rBV	66212	194677	21.30%	2.968%
16	4.690	589	591	595	rVB	800	892	0.10%	0.014%
17	4.733	596	598	600	rVB	707	550	0.06%	0.008%
18	5.068	642	653	667	rBV	123596	362633	39.68%	5.529%
19	5.239	679	681	685	rBV	852	1194	0.13%	0.018%
20	5.306	690	692	695	rVB	764	841	0.09%	0.013%
21	5.336	695	697	700	rBV	627	691	0.08%	0.011%
22	5.562	730	734	737	rBV	1059	1780	0.19%	0.027%
23	5.775	764	769	771	rBV2	462	784	0.09%	0.012%
24	5.849	778	781	786	rVB	588	977	0.11%	0.015%
25	5.977	789	802	822	rVV2	307408	913858	100.00%	13.935%
26	6.190	835	837	840	rVB	750	734	0.08%	0.011%
27	6.233	840	844	845	rBV2	415	467	0.05%	0.007%
28	6.367	862	866	867	rBV2	480	556	0.06%	0.008%
29	6.513	888	890	893	rVB2	747	674	0.07%	0.010%
30	6.562	893	898	901	rBV2	632	1252	0.14%	0.019%
31	6.763	922	931	944	rBV	193342	464532	50.83%	7.083%
32	7.110	982	988	996	rBV5	4186	10622	1.16%	0.162%
33	7.312	1012	1021	1032	rVV	190328	413002	45.19%	6.297%
34	7.848	1108	1109	1111	rBV	892	475	0.05%	0.007%
35	7.866	1111	1112	1116	rVV	635	650	0.07%	0.010%
36	7.940	1123	1124	1127	rVB	911	832	0.09%	0.013%

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 ClientSampleId :  
 GBCC4

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122821WMA.M  
 Title : VOC Analysis

37	8.141	1154	1157	1158	rBV	621	541	0.06%	0.008%
38	8.190	1163	1165	1169	rVV	604	804	0.09%	0.012%
39	8.251	1173	1175	1179	rBV2	587	859	0.09%	0.013%
40	8.330	1181	1188	1199	rBV	131536	217315	23.78%	3.314%
41	8.507	1215	1217	1219	rVB	632	533	0.06%	0.008%
42	8.531	1219	1221	1222	rBV	598	472	0.05%	0.007%
43	8.653	1234	1241	1248	rBV	469953	714616	78.20%	10.896%
44	8.720	1249	1252	1257	rVB	8186	12276	1.34%	0.187%
45	8.891	1277	1280	1282	rBV	497	484	0.05%	0.007%
46	8.952	1284	1290	1300	rVV	92311	137572	15.05%	2.098%
47	9.074	1308	1310	1313	rVB	519	522	0.06%	0.008%
48	9.183	1325	1328	1329	rBV	890	690	0.08%	0.011%
49	9.281	1336	1344	1349	rBV4	1203	2572	0.28%	0.039%
50	9.324	1349	1351	1352	rBV2	691	513	0.06%	0.008%
51	9.391	1356	1362	1376	rVB	278871	416118	45.53%	6.345%
52	9.537	1383	1386	1387	rBV3	661	703	0.08%	0.011%
53	9.610	1394	1398	1399	rBV	436	494	0.05%	0.008%
54	9.659	1405	1406	1409	rVB	684	482	0.05%	0.007%
55	9.683	1409	1410	1411	rBV	820	498	0.05%	0.008%
56	9.744	1419	1420	1424	rVB2	584	628	0.07%	0.010%
57	9.823	1430	1433	1436	rVB	591	750	0.08%	0.011%
58	9.994	1459	1461	1463	rBV	616	567	0.06%	0.009%
59	10.055	1465	1471	1483	rBV	392912	533015	58.33%	8.127%
60	10.305	1508	1512	1515	rVB4	2252	2953	0.32%	0.045%
61	10.646	1564	1568	1574	rVB4	1338	2388	0.26%	0.036%
62	10.756	1584	1586	1589	rVB	1001	866	0.09%	0.013%
63	11.012	1625	1628	1629	rBV	636	558	0.06%	0.009%
64	11.043	1629	1633	1635	rVV2	504	653	0.07%	0.010%
65	11.122	1642	1646	1651	rVB3	4129	6166	0.67%	0.094%
66	11.195	1652	1658	1667	rVV	311005	397658	43.51%	6.064%
67	11.390	1686	1690	1698	rVB4	901	1800	0.20%	0.027%
68	11.457	1698	1701	1702	rBV2	883	1042	0.11%	0.016%
69	11.476	1702	1704	1708	rVB2	1663	1797	0.20%	0.027%
70	11.750	1746	1749	1754	rVB3	4847	6606	0.72%	0.101%
71	11.939	1776	1780	1782	rVV3	1511	2072	0.23%	0.032%
72	11.975	1783	1786	1789	rVV2	1359	1198	0.13%	0.018%
73	12.024	1789	1794	1804	rVV	385506	473770	51.84%	7.224%
74	12.323	1837	1843	1850	rVB	453925	581250	63.60%	8.863%
75	12.427	1857	1860	1864	rBV3	1477	2147	0.23%	0.033%
76	12.664	1897	1899	1900	rBV	652	484	0.05%	0.007%

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Integration Parameters: LSCINT.P

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 Start Thrs: 0.2 Max Peaks: 100  
 Stop Thrs : 0 Peak Location: TOP

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 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXML122821WMA.M  
 Title : VOC Analysis

77	12.927	1940	1942	1943	rVB	899	587	0.06%	0.009%
78	12.945	1943	1945	1948	rBV	713	790	0.09%	0.012%
79	13.055	1960	1963	1967	rVB2	1451	1364	0.15%	0.021%
80	13.189	1982	1985	1986	rBV	569	564	0.06%	0.009%
81	13.207	1986	1988	1991	rVV2	624	711	0.08%	0.011%
82	13.536	2040	2042	2045	rBV	587	696	0.08%	0.011%
83	13.561	2045	2046	2048	rBV2	743	558	0.06%	0.009%
84	13.591	2048	2051	2056	rVB3	2260	2922	0.32%	0.045%
85	13.780	2079	2082	2084	rBV3	1381	1872	0.20%	0.029%
86	13.859	2093	2095	2098	rVB2	563	525	0.06%	0.008%
87	13.957	2110	2111	2114	rVB3	1061	861	0.09%	0.013%
88	14.115	2133	2137	2139	rVV	627	898	0.10%	0.014%
89	14.195	2149	2150	2152	rBV	707	544	0.06%	0.008%
90	14.609	2216	2218	2220	rBV	451	526	0.06%	0.008%
91	14.640	2220	2223	2228	rVV4	2449	3771	0.41%	0.058%
92	14.871	2259	2261	2264	rBV	654	796	0.09%	0.012%
93	15.188	2311	2313	2316	rVB	728	593	0.06%	0.009%
94	15.359	2337	2341	2342	rBV2	564	700	0.08%	0.011%
95	15.469	2357	2359	2360	rBV2	659	459	0.05%	0.007%
96	15.658	2388	2390	2394	rVB2	867	736	0.08%	0.011%
97	15.731	2400	2402	2405	rVB3	865	735	0.08%	0.011%
98	16.030	2448	2451	2452	rBV2	424	496	0.05%	0.008%
99	16.347	2500	2503	2504	rBV3	946	785	0.09%	0.012%
100	16.597	2542	2544	2545	rBV	1183	926	0.10%	0.014%

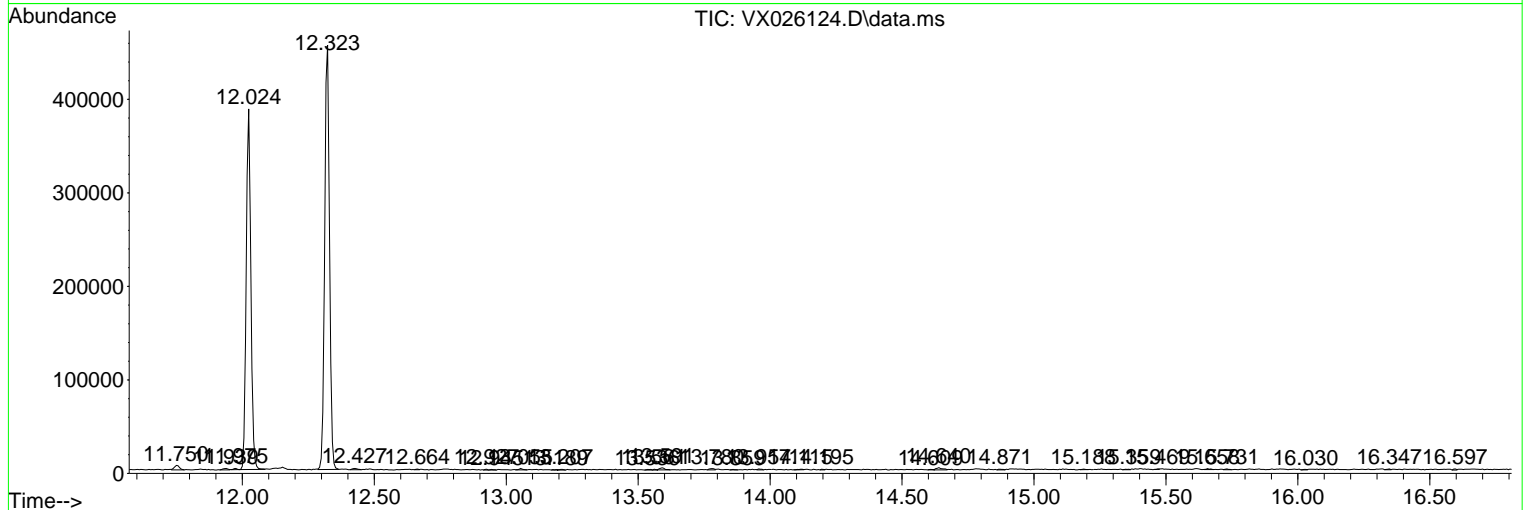
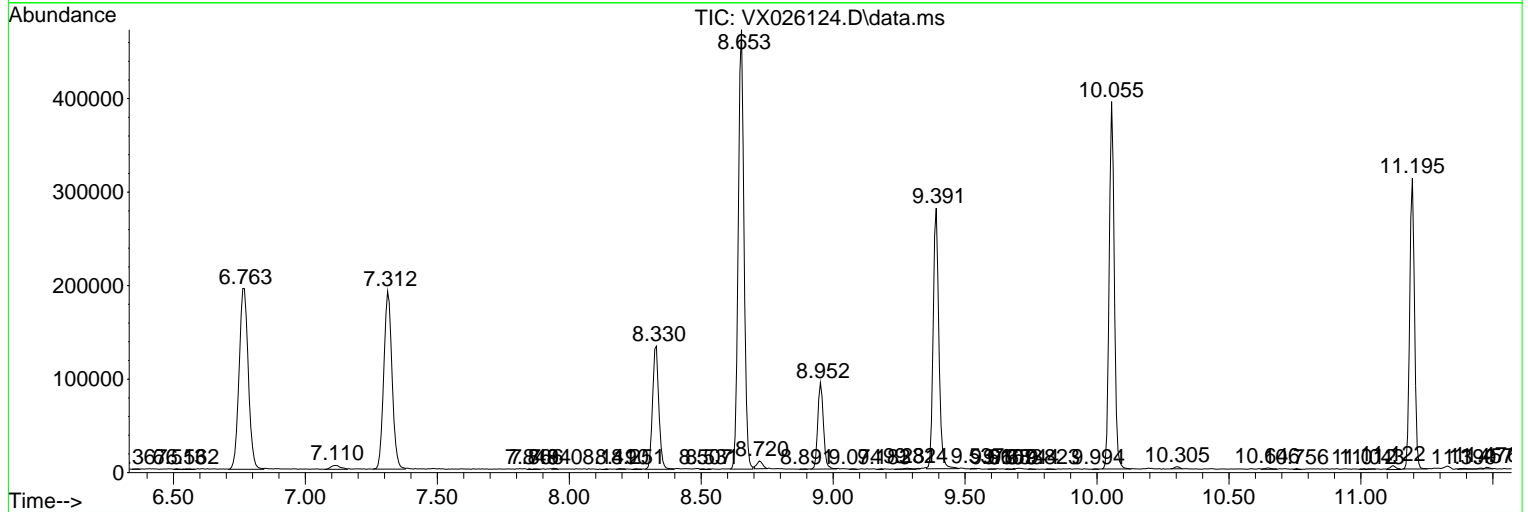
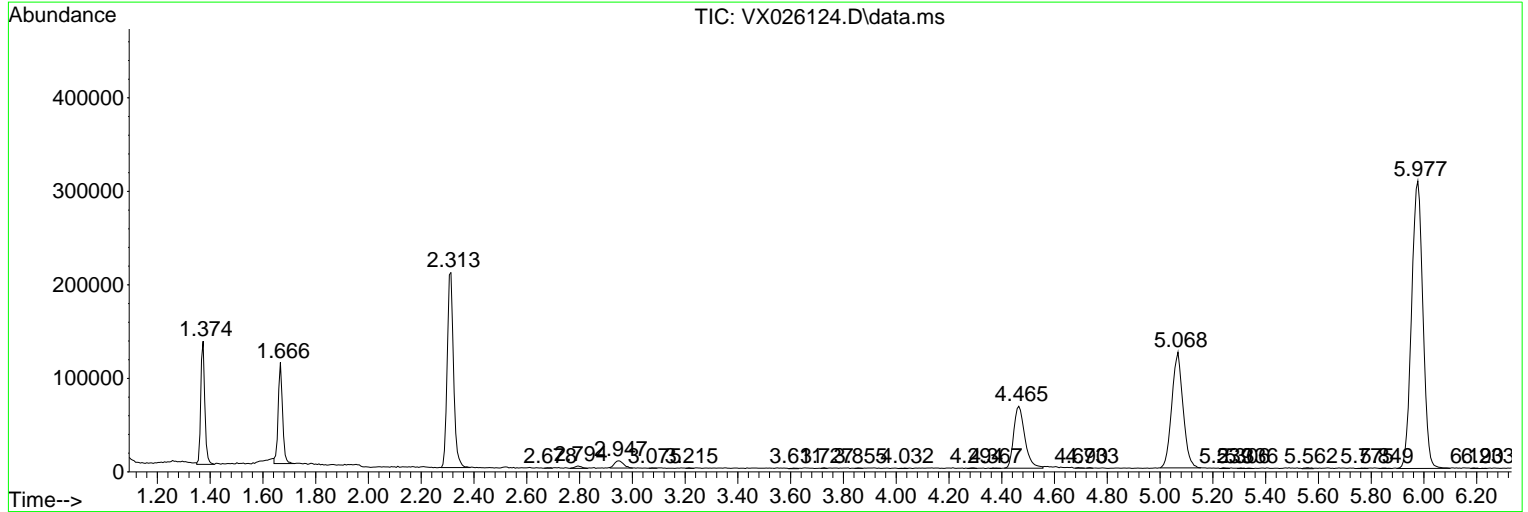
Sum of corrected areas: 6558219

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 ALS Vial : 31 Sample Multiplier: 1

Instrument :  
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 ClientSampleId :  
 GBCC4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\SFAMXLM122821WMA.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\SFAMXML122821WMA.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\SFAMXLM122821WMA.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

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