

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122721\
 Data File : VX026073.D
 Acq On : 27 Dec 2021 19:36
 Operator : JC/MD
 Sample : M5174-06ME
 Misc : 5.66g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBC17ME

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\SFAMXML122321WMA.M
 Title : VOC Analysis

Signal : TIC: VX026073.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	27	29	31	rVB	1747	1410	0.17%	0.023%
2	1.374	43	47	54	rVB	104455	119077	14.28%	1.943%
3	1.550	74	76	77	rBV2	765	645	0.08%	0.011%
4	1.642	82	91	92	rBV2	8643	15446	1.85%	0.252%
5	1.672	92	96	102	rVB	54772	79262	9.50%	1.293%
6	2.190	179	181	184	rVB3	992	1005	0.12%	0.016%
7	2.294	191	198	205	rBV	183981	288338	34.57%	4.704%
8	2.501	230	232	235	rVB2	459	388	0.05%	0.006%
9	2.690	259	263	264	rBV3	377	495	0.06%	0.008%
10	2.721	264	268	274	rVB3	696	1338	0.16%	0.022%
11	2.788	274	279	286	rVB4	2415	5108	0.61%	0.083%
12	2.940	301	304	305	rBV2	1082	1227	0.15%	0.020%
13	3.172	340	342	346	rVB3	412	610	0.07%	0.010%
14	3.233	351	352	357	rBV2	378	497	0.06%	0.008%
15	3.324	363	367	369	rBV	367	482	0.06%	0.008%
16	3.562	403	406	409	rVV2	382	415	0.05%	0.007%
17	3.660	419	422	425	rBV2	355	511	0.06%	0.008%
18	4.178	505	507	512	rVB2	212	399	0.05%	0.007%
19	4.489	546	558	590	rBV2	35300	180737	21.67%	2.949%
20	4.714	593	595	597	rBV3	626	468	0.06%	0.008%
21	5.068	638	653	668	rBV	105522	325582	39.03%	5.312%
22	5.519	724	727	729	rBV3	362	393	0.05%	0.006%
23	5.970	789	801	819	rBV2	295383	834105	100.00%	13.608%
24	6.367	860	866	871	rBV4	597	1513	0.18%	0.025%
25	6.403	871	872	875	rVB2	414	390	0.05%	0.006%
26	6.763	922	931	943	rBV	188582	459261	55.06%	7.492%
27	7.110	981	988	995	rBV6	3184	7447	0.89%	0.121%
28	7.202	1000	1003	1006	rBV2	583	977	0.12%	0.016%
29	7.312	1012	1021	1035	rVV	167025	372123	44.61%	6.071%
30	7.488	1046	1050	1053	rBV3	668	1032	0.12%	0.017%
31	7.811	1097	1103	1105	rBV3	276	376	0.05%	0.006%
32	7.927	1120	1122	1124	rBV2	349	369	0.04%	0.006%
33	8.141	1154	1157	1158	rBV	716	774	0.09%	0.013%
34	8.159	1158	1160	1164	rVB	1033	1138	0.14%	0.019%
35	8.330	1182	1188	1196	rBV	83152	146382	17.55%	2.388%
36	8.494	1210	1215	1217	rVB3	486	665	0.08%	0.011%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
 Title : VOC Analysis

37	8.513	1217	1218	1222	rVB	480	376	0.05%	0.006%
38	8.653	1232	1241	1249	rBV	411243	661268	79.28%	10.788%
39	8.720	1249	1252	1266	rVB2	6089	11659	1.40%	0.190%
40	8.866	1269	1276	1277	rBV2	715	864	0.10%	0.014%
41	8.903	1279	1282	1285	rVV4	1867	2775	0.33%	0.045%
42	8.951	1285	1290	1301	rVB	53026	87326	10.47%	1.425%
43	9.128	1317	1319	1322	rVB2	396	405	0.05%	0.007%
44	9.275	1338	1343	1347	rBV3	3353	5790	0.69%	0.094%
45	9.336	1347	1353	1356	rVV3	2439	5730	0.69%	0.093%
46	9.415	1357	1366	1380	rVV	160308	382146	45.82%	6.234%
47	9.543	1383	1387	1393	rVV5	2424	4219	0.51%	0.069%
48	9.604	1395	1397	1400	rVB	549	619	0.07%	0.010%
49	9.720	1413	1416	1424	rVB4	816	1484	0.18%	0.024%
50	9.854	1431	1438	1441	rBV4	1053	2250	0.27%	0.037%
51	10.055	1465	1471	1486	rVV	370562	548452	65.75%	8.947%
52	10.195	1491	1494	1496	rBV2	1051	1186	0.14%	0.019%
53	10.311	1508	1513	1517	rVB3	1837	2869	0.34%	0.047%
54	10.366	1519	1522	1525	rVV4	317	519	0.06%	0.008%
55	10.555	1551	1553	1556	rBV2	597	490	0.06%	0.008%
56	10.658	1563	1570	1573	rVV5	635	1152	0.14%	0.019%
57	10.719	1577	1580	1583	rVV5	344	484	0.06%	0.008%
58	10.756	1583	1586	1592	rVV5	478	771	0.09%	0.013%
59	10.835	1597	1599	1602	rVB2	506	492	0.06%	0.008%
60	10.908	1607	1611	1612	rBV2	417	405	0.05%	0.007%
61	10.976	1620	1622	1627	rVB4	610	739	0.09%	0.012%
62	11.024	1627	1630	1632	rBV2	491	592	0.07%	0.010%
63	11.116	1641	1645	1652	rVB2	3995	5851	0.70%	0.095%
64	11.201	1652	1659	1665	rBV	265662	361055	43.29%	5.890%
65	11.250	1665	1667	1669	rVB3	571	379	0.05%	0.006%
66	11.329	1673	1680	1685	rVB2	5736	10250	1.23%	0.167%
67	11.378	1685	1688	1690	rBV3	1209	1416	0.17%	0.023%
68	11.475	1699	1704	1709	rBV7	1974	4018	0.48%	0.066%
69	11.542	1713	1715	1718	rVB4	765	781	0.09%	0.013%
70	11.634	1728	1730	1733	rVB4	591	507	0.06%	0.008%
71	11.713	1741	1743	1745	rBV4	784	565	0.07%	0.009%
72	11.750	1745	1749	1757	rVB3	5588	8302	1.00%	0.135%
73	11.847	1762	1765	1767	rBV3	1037	1128	0.14%	0.018%
74	11.933	1775	1779	1783	rBV3	2163	3430	0.41%	0.056%
75	11.975	1783	1786	1789	rBV5	920	999	0.12%	0.016%
76	12.024	1789	1794	1800	rBV	421130	554827	66.52%	9.051%

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 Title : VOC Analysis

77	12.146	1813	1814	1818	rVB2	3191	3080	0.37%	0.050%
78	12.237	1827	1829	1831	rBV3	809	674	0.08%	0.011%
79	12.323	1835	1843	1850	rBV	454808	570385	68.38%	9.305%
80	12.426	1858	1860	1864	rVB3	2043	2276	0.27%	0.037%
81	12.768	1913	1916	1920	rBV2	2894	3283	0.39%	0.054%
82	12.951	1943	1946	1947	rBV3	1180	1296	0.16%	0.021%
83	13.042	1957	1961	1962	rBV3	1794	2491	0.30%	0.041%
84	13.365	2013	2014	2016	rBV2	1332	1046	0.13%	0.017%
85	15.182	2310	2312	2314	rBV3	1390	1263	0.15%	0.021%
86	15.402	2343	2348	2353	rVB8	1497	2983	0.36%	0.049%
87	15.591	2377	2379	2381	rBV2	772	713	0.09%	0.012%
88	15.609	2381	2382	2383	rVV	1272	780	0.09%	0.013%
89	15.651	2387	2389	2393	rVB5	1381	1636	0.20%	0.027%
90	15.731	2401	2402	2405	rVB3	691	478	0.06%	0.008%
91	15.810	2414	2415	2417	rBV2	772	572	0.07%	0.009%
92	15.834	2417	2419	2422	rVV4	663	498	0.06%	0.008%
93	16.090	2460	2461	2466	rVB4	971	1125	0.13%	0.018%
94	16.151	2466	2471	2475	rBV4	598	1227	0.15%	0.020%
95	16.231	2482	2484	2487	rBV4	566	668	0.08%	0.011%
96	16.267	2488	2490	2493	rVV4	585	653	0.08%	0.011%
97	16.359	2503	2505	2514	rVB7	931	1586	0.19%	0.026%
98	16.468	2522	2523	2525	rVB2	819	521	0.06%	0.008%
99	16.499	2525	2528	2529	rBV2	765	796	0.10%	0.013%
100	16.535	2532	2534	2536	rVB	1017	722	0.09%	0.012%

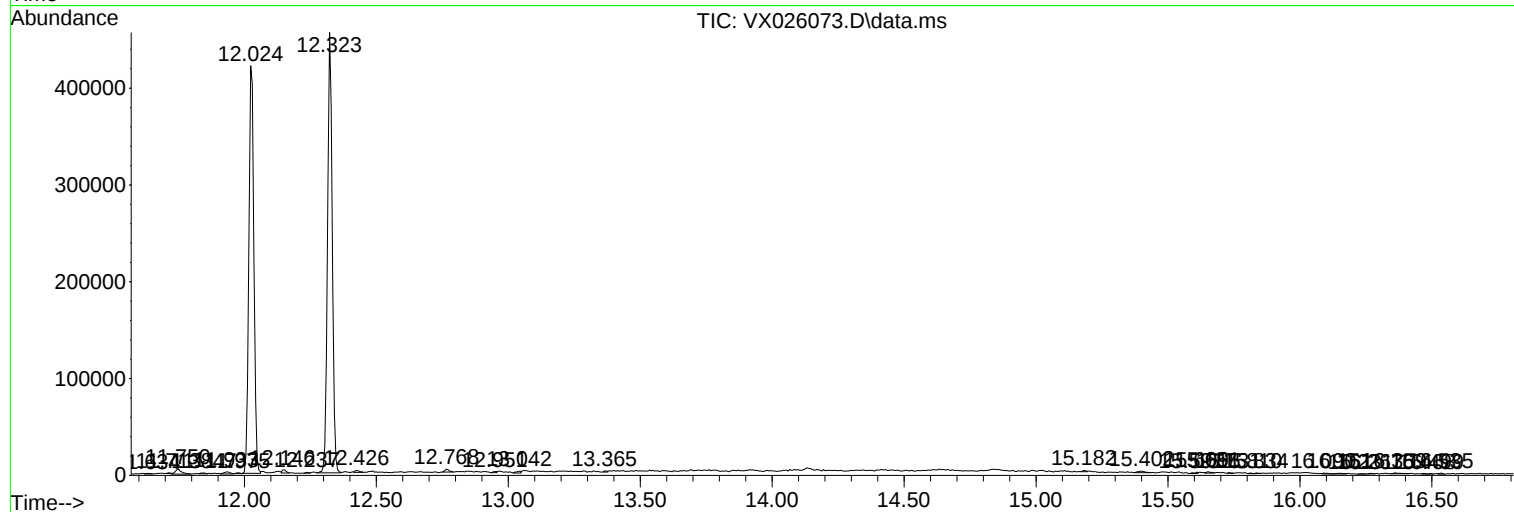
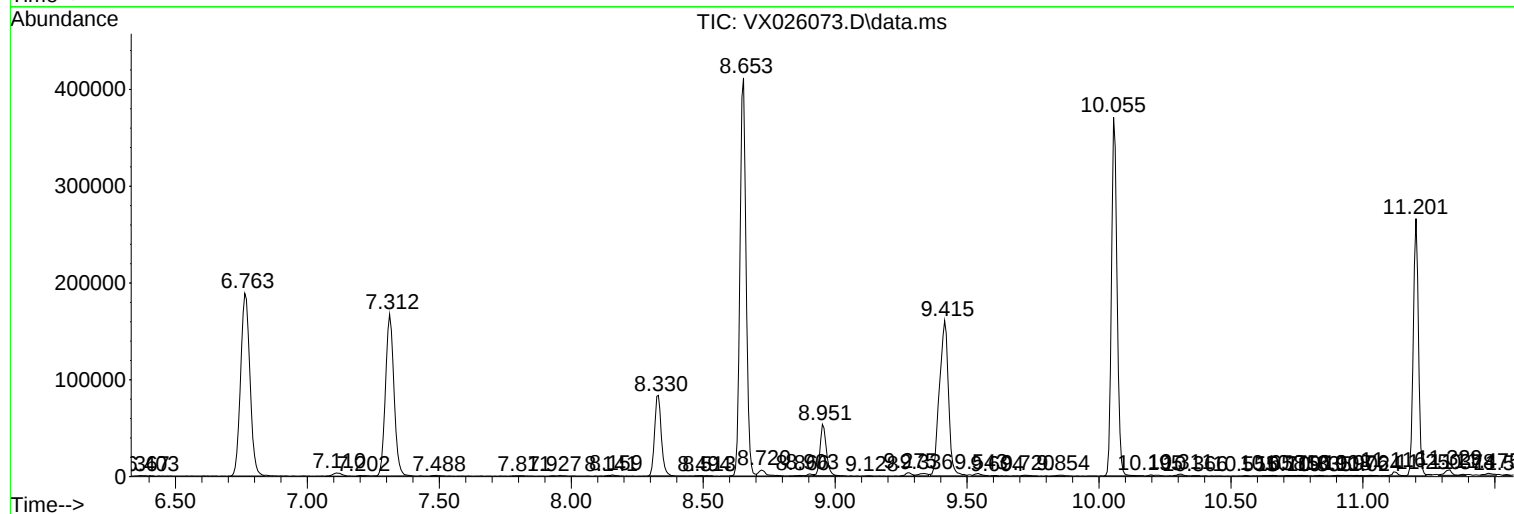
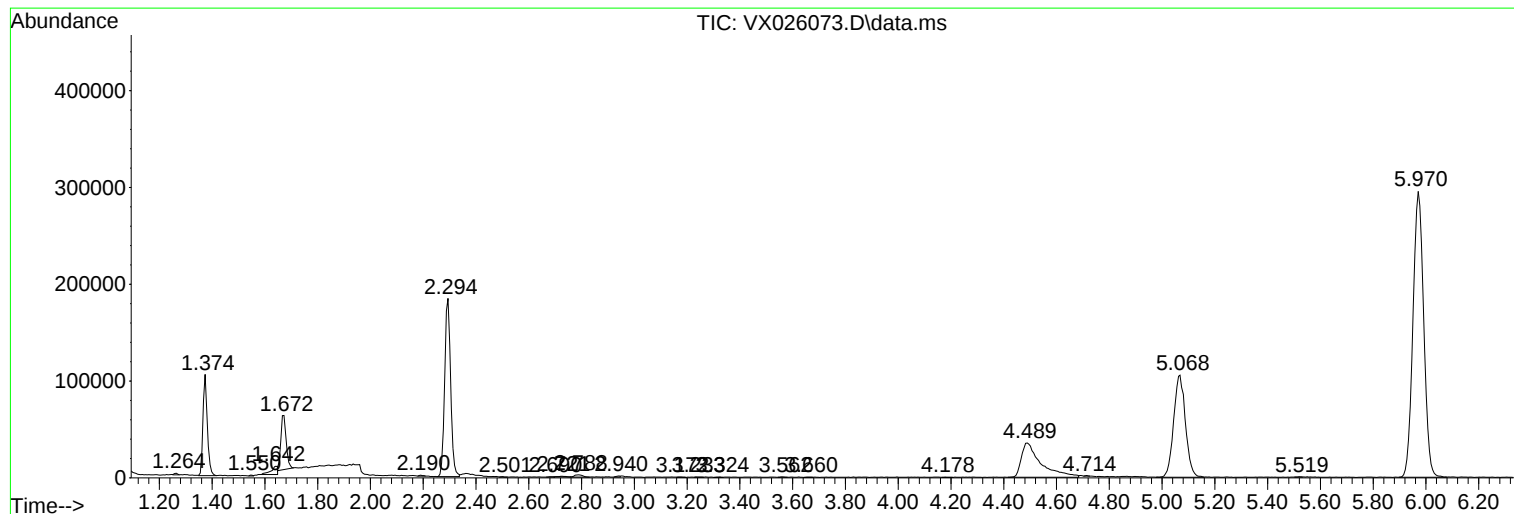
Sum of corrected areas: 6129707

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM122321WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_X
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GBC17ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML122321WMA.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\SFAMXML122321WMA.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