

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039406.D
 Acq On : 20 Dec 2023 16:59
 Operator : JC/MD
 Sample : 05794-21ME
 Misc : 5.89g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGRG2ME

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: VX039406.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	43	46	61	rBV	65950	110514	12.50%	1.664%
2	1.648	89	92	97	rBV	23636	34995	3.96%	0.527%
3	2.288	190	197	206	rBV	175417	285271	32.27%	4.296%
4	2.489	228	230	236	rVB2	644	861	0.10%	0.013%
5	2.709	263	266	267	rBV2	604	599	0.07%	0.009%
6	2.788	274	279	285	rBV4	2311	5136	0.58%	0.077%
7	2.941	297	304	315	rBV	5778	14862	1.68%	0.224%
8	3.428	380	384	387	rVB3	686	1053	0.12%	0.016%
9	3.690	425	427	430	rBV2	181	274	0.03%	0.004%
10	3.831	447	450	454	rBV	251	304	0.03%	0.005%
11	3.934	465	467	471	rBV	190	270	0.03%	0.004%
12	4.477	547	556	589	rBV	44964	217928	24.65%	3.282%
13	5.056	639	651	668	rVV	110448	351877	39.81%	5.299%
14	5.458	713	717	721	rBV2	431	760	0.09%	0.011%
15	5.544	729	731	734	rBV2	223	276	0.03%	0.004%
16	5.861	780	783	785	rVV2	213	259	0.03%	0.004%
17	5.964	787	800	825	rVV2	299694	883915	100.00%	13.311%
18	6.373	861	867	868	rBV3	1082	1611	0.18%	0.024%
19	6.501	886	888	890	rBV	292	327	0.04%	0.005%
20	6.556	894	897	900	rVV2	236	316	0.04%	0.005%
21	6.598	900	904	907	rVV	412	523	0.06%	0.008%
22	6.629	907	909	913	rVB3	223	267	0.03%	0.004%
23	6.757	921	930	946	rBV	192888	476509	53.91%	7.176%
24	6.952	960	962	967	rVB2	374	458	0.05%	0.007%
25	7.123	982	990	998	rBV9	1891	5677	0.64%	0.085%
26	7.208	999	1004	1011	rVV5	2044	5830	0.66%	0.088%
27	7.306	1012	1020	1039	rVB	176535	401139	45.38%	6.041%
28	7.489	1046	1050	1054	rVB4	607	1109	0.13%	0.017%
29	7.976	1123	1130	1139	rVB6	1811	4134	0.47%	0.062%
30	8.098	1145	1150	1156	rVB4	1805	3842	0.43%	0.058%
31	8.257	1173	1176	1178	rVV2	403	472	0.05%	0.007%
32	8.324	1181	1187	1200	rVV	108113	189426	21.43%	2.853%
33	8.434	1203	1205	1210	rVB3	508	686	0.08%	0.010%
34	8.507	1214	1217	1219	rBV2	303	285	0.03%	0.004%
35	8.647	1234	1240	1250	rBV	414502	668011	75.57%	10.059%
36	8.952	1285	1290	1305	rVV	74942	122972	13.91%	1.852%

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Integrator: RTE

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Peak Location: TOP

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

37	9.061	1306	1308	1310	rVB2	441	318	0.04%	0.005%
38	9.116	1316	1317	1319	rBV	443	274	0.03%	0.004%
39	9.269	1340	1342	1348	rVB4	404	808	0.09%	0.012%
40	9.397	1357	1363	1380	rBV	257888	491035	55.55%	7.394%
41	9.659	1404	1406	1409	rBV3	445	463	0.05%	0.007%
42	9.714	1411	1415	1422	rBV3	996	1804	0.20%	0.027%
43	9.848	1434	1437	1439	rBV	307	352	0.04%	0.005%
44	9.897	1443	1445	1453	rVB3	359	586	0.07%	0.009%
45	10.012	1461	1464	1465	rBV	345	309	0.03%	0.005%
46	10.055	1465	1471	1483	rBV	390110	572472	64.77%	8.621%
47	10.305	1509	1512	1518	rBV2	2371	3613	0.41%	0.054%
48	10.464	1534	1538	1542	rVB2	448	589	0.07%	0.009%
49	10.567	1551	1555	1556	rBV2	449	559	0.06%	0.008%
50	10.647	1565	1568	1575	rVB4	1635	2435	0.28%	0.037%
51	10.762	1582	1587	1588	rBV3	594	756	0.09%	0.011%
52	10.811	1593	1595	1600	rBV4	1079	1520	0.17%	0.023%
53	10.854	1600	1602	1605	rVV2	664	738	0.08%	0.011%
54	10.890	1605	1608	1612	rVV5	1180	1754	0.20%	0.026%
55	10.945	1612	1617	1622	rVB	11458	15872	1.80%	0.239%
56	11.025	1627	1630	1636	rVB4	955	1448	0.16%	0.022%
57	11.079	1636	1639	1642	rBV4	731	1058	0.12%	0.016%
58	11.122	1642	1646	1651	rBV3	6181	10667	1.21%	0.161%
59	11.195	1651	1658	1669	rVB	317967	410657	46.46%	6.184%
60	11.390	1686	1690	1694	rVB3	2439	3211	0.36%	0.048%
61	11.482	1698	1705	1713	rVB6	6948	14894	1.69%	0.224%
62	11.573	1718	1720	1721	rBV2	417	339	0.04%	0.005%
63	11.689	1735	1739	1740	rBV2	1529	1904	0.22%	0.029%
64	11.750	1746	1749	1757	rVB3	3319	6928	0.78%	0.104%
65	11.835	1759	1763	1765	rBV4	907	1318	0.15%	0.020%
66	11.884	1768	1771	1775	rVB5	1725	2146	0.24%	0.032%
67	11.933	1775	1779	1783	rBV2	5397	7806	0.88%	0.118%
68	11.969	1783	1785	1788	rVB2	2121	2299	0.26%	0.035%
69	12.024	1789	1794	1804	rBV	458332	596706	67.51%	8.986%
70	12.250	1826	1831	1837	rBV5	1974	4154	0.47%	0.063%
71	12.323	1837	1843	1851	rVV	461163	594957	67.31%	8.959%
72	12.421	1857	1859	1863	rVB4	3619	3942	0.45%	0.059%
73	12.457	1863	1865	1867	rBV2	713	605	0.07%	0.009%
74	12.518	1873	1875	1876	rBV	399	301	0.03%	0.005%
75	12.762	1910	1915	1919	rBV2	4558	6478	0.73%	0.098%
76	13.006	1951	1955	1958	rVV4	1444	2230	0.25%	0.034%

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Title : VOC Analysis

77	13.049	1959	1962	1967	rVB4	2320	3785	0.43%	0.057%
78	13.158	1978	1980	1984	rBV4	621	723	0.08%	0.011%
79	13.262	1995	1997	2000	rBV3	1949	2351	0.27%	0.035%
80	13.384	2013	2017	2020	rVB5	700	841	0.10%	0.013%
81	13.542	2041	2043	2044	rBV2	542	357	0.04%	0.005%
82	13.591	2048	2051	2055	rVB6	3003	3837	0.43%	0.058%
83	13.683	2061	2066	2072	rBV5	3676	5822	0.66%	0.088%
84	13.780	2077	2082	2089	rVV2	8765	13295	1.50%	0.200%
85	13.841	2089	2092	2099	rVB5	1451	2238	0.25%	0.034%
86	13.963	2109	2112	2115	rBV4	1471	1751	0.20%	0.026%
87	14.036	2121	2124	2127	rBV2	1564	1802	0.20%	0.027%
88	14.134	2137	2140	2145	rVB3	4030	5067	0.57%	0.076%
89	14.292	2164	2166	2167	rBV	577	410	0.05%	0.006%
90	14.359	2174	2177	2178	rBV3	666	754	0.09%	0.011%
91	14.396	2180	2183	2187	rVB2	3156	3879	0.44%	0.058%
92	14.640	2219	2223	2227	rVB2	4924	6497	0.74%	0.098%
93	14.756	2238	2242	2243	rBV3	1794	2337	0.26%	0.035%
94	14.780	2243	2246	2251	rVB2	5736	7617	0.86%	0.115%
95	15.213	2313	2317	2319	rBV3	2665	3142	0.36%	0.047%
96	15.609	2380	2382	2387	rBV3	2561	3053	0.35%	0.046%
97	15.810	2411	2415	2416	rBV4	1299	1884	0.21%	0.028%
98	15.950	2437	2438	2440	rBV2	1043	1006	0.11%	0.015%
99	16.328	2496	2500	2508	rVB5	2436	4706	0.53%	0.071%
100	16.402	2511	2512	2514	rBV2	441	441	0.05%	0.007%

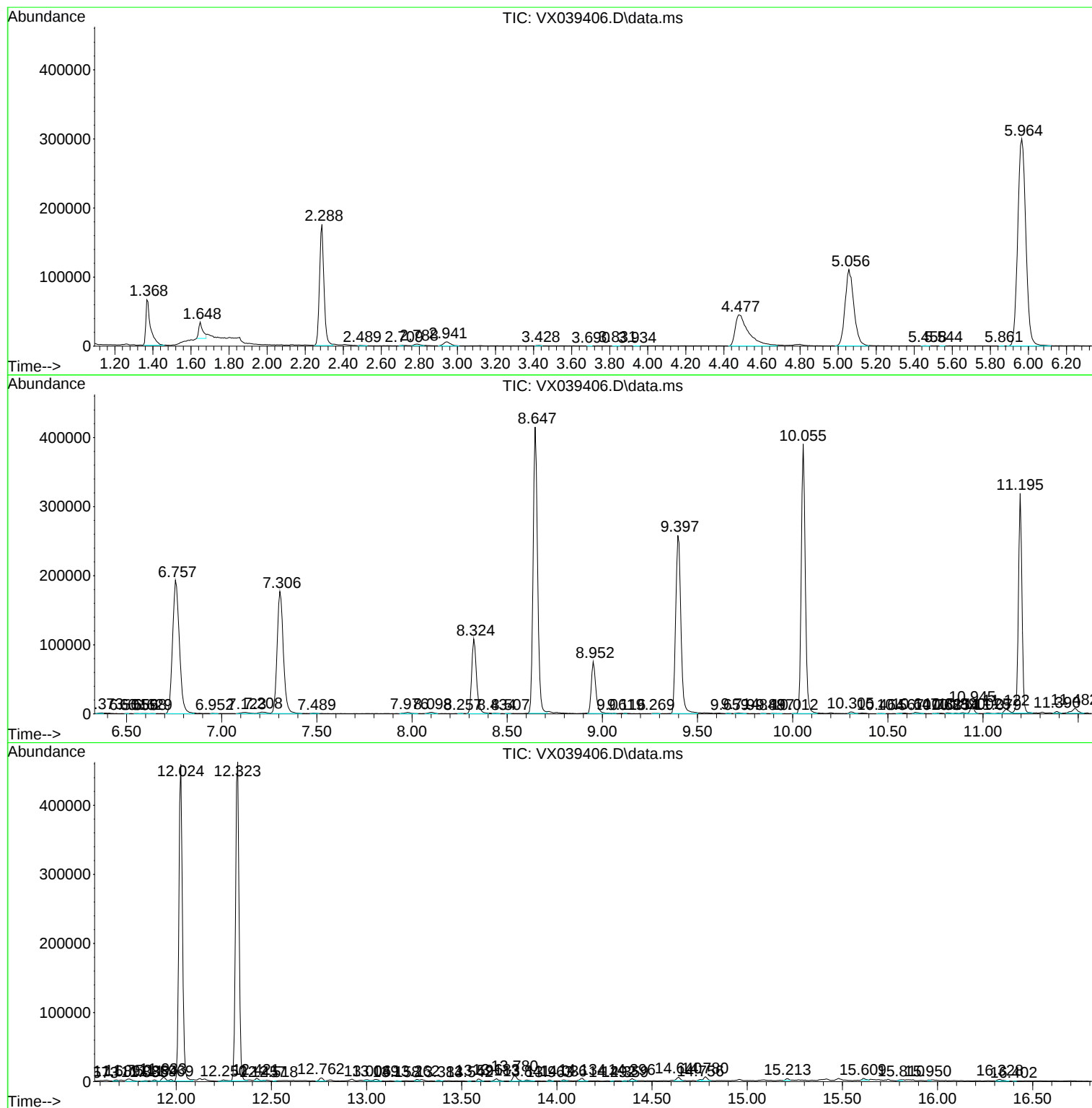
Sum of corrected areas: 6640648

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Instrument :
MSVOA_X
ClientSampleId :
BGRG2ME

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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MSVOA_X
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BGRG2ME

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