

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121021\
 Data File : VX025694.D
 Acq On : 10 Dec 2021 12:21
 Operator : JC/MD
 Sample : M5004-04ME
 Misc : 6.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKW3ME

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\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025694.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	55	rVB	42806	50868	12.14%	1.494%
2	1.648	88	92	98	rBV	33224	41245	9.85%	1.212%
3	2.282	190	196	205	rBV	86446	140810	33.62%	4.136%
4	2.563	241	242	244	rBV	516	350	0.08%	0.010%
5	2.678	259	261	262	rBV2	401	292	0.07%	0.009%
6	2.776	275	277	286	rVB3	1621	3044	0.73%	0.089%
7	2.947	298	305	313	rBV2	2986	7723	1.84%	0.227%
8	3.221	348	350	353	rBV2	266	218	0.05%	0.006%
9	3.794	442	444	449	rBV2	262	388	0.09%	0.011%
10	3.831	449	450	453	rBV	293	223	0.05%	0.007%
11	4.007	478	479	481	rVB	396	203	0.05%	0.006%
12	4.294	525	526	529	rBV2	309	328	0.08%	0.010%
13	4.410	543	545	547	rVB	305	199	0.05%	0.006%
14	4.483	547	557	579	rBV	15923	70132	16.74%	2.060%
15	5.062	640	652	669	rVB3	43417	157795	37.67%	4.635%
16	5.367	698	702	703	rBV2	538	764	0.18%	0.022%
17	5.440	712	714	715	rBV	382	252	0.06%	0.007%
18	5.849	778	781	782	rBV	209	219	0.05%	0.006%
19	5.964	789	800	819	rVB2	131109	382858	91.40%	11.247%
20	6.355	860	864	872	rBV5	1177	2694	0.64%	0.079%
21	6.525	890	892	894	rBV	388	349	0.08%	0.010%
22	6.763	920	931	948	rBV	137050	347757	83.02%	10.216%
23	6.928	956	958	960	rVB2	379	244	0.06%	0.007%
24	7.117	982	989	997	rVB6	1930	5222	1.25%	0.153%
25	7.208	997	1004	1012	rBV4	795	2444	0.58%	0.072%
26	7.312	1012	1021	1033	rBV	74996	171821	41.02%	5.047%
27	7.543	1056	1059	1060	rBV2	348	292	0.07%	0.009%
28	7.610	1068	1070	1073	rBV2	229	271	0.06%	0.008%
29	7.867	1110	1112	1115	rVB	360	313	0.07%	0.009%
30	7.909	1115	1119	1120	rBV2	287	327	0.08%	0.010%
31	8.080	1146	1147	1149	rBV	317	243	0.06%	0.007%
32	8.141	1154	1157	1160	rVB	215	266	0.06%	0.008%
33	8.232	1169	1172	1173	rVB	322	226	0.05%	0.007%
34	8.245	1173	1174	1178	rBV2	253	334	0.08%	0.010%
35	8.330	1181	1188	1197	rBV	50754	91384	21.82%	2.685%
36	8.555	1223	1225	1227	rBV2	226	267	0.06%	0.008%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	8.647	1234	1240	1248	rVV	198599	327827	78.26%	9.630%
38	8.720	1249	1252	1257	rVB3	2583	4089	0.98%	0.120%
39	8.799	1263	1265	1267	rVB	340	212	0.05%	0.006%
40	8.952	1285	1290	1298	rBV	33271	56911	13.59%	1.672%
41	9.092	1309	1313	1316	rVB2	240	302	0.07%	0.009%
42	9.275	1337	1343	1352	rVB	37955	56674	13.53%	1.665%
43	9.397	1357	1363	1375	rBV	93922	153350	36.61%	4.505%
44	9.555	1388	1389	1393	rVB2	406	458	0.11%	0.013%
45	9.592	1393	1395	1398	rBV2	258	295	0.07%	0.009%
46	9.665	1406	1407	1411	rVB	256	243	0.06%	0.007%
47	9.708	1411	1414	1416	rBV2	456	560	0.13%	0.016%
48	9.854	1437	1438	1441	rBV	336	299	0.07%	0.009%
49	9.903	1444	1446	1449	rBV	192	211	0.05%	0.006%
50	10.006	1461	1463	1465	rBV2	352	285	0.07%	0.008%
51	10.055	1465	1471	1479	rBV	284947	418881	100.00%	12.305%
52	10.195	1492	1494	1497	rVB2	399	358	0.09%	0.011%
53	10.299	1506	1511	1517	rVB3	480	1153	0.28%	0.034%
54	10.378	1521	1524	1525	rBV2	221	279	0.07%	0.008%
55	10.451	1535	1536	1539	rVB2	242	244	0.06%	0.007%
56	10.488	1539	1542	1543	rBV	303	279	0.07%	0.008%
57	10.665	1570	1571	1573	rBV	330	294	0.07%	0.009%
58	10.720	1579	1580	1582	rBV	322	243	0.06%	0.007%
59	10.829	1595	1598	1600	rBV	268	342	0.08%	0.010%
60	11.122	1643	1646	1650	rVB2	1664	2103	0.50%	0.062%
61	11.195	1653	1658	1667	rVB	135642	175715	41.95%	5.162%
62	11.256	1667	1668	1669	rBV	290	209	0.05%	0.006%
63	11.421	1694	1695	1698	rVB2	395	270	0.06%	0.008%
64	11.451	1698	1700	1701	rBV	309	280	0.07%	0.008%
65	11.555	1713	1717	1718	rBV	169	234	0.06%	0.007%
66	11.689	1737	1739	1742	rVV	493	394	0.09%	0.012%
67	11.744	1745	1748	1756	rVB3	1424	2124	0.51%	0.062%
68	11.902	1771	1774	1775	rBV2	182	219	0.05%	0.006%
69	11.939	1775	1780	1784	rVV3	897	1459	0.35%	0.043%
70	12.024	1789	1794	1804	rBV	339615	415176	99.12%	12.196%
71	12.128	1808	1811	1812	rBV2	729	869	0.21%	0.026%
72	12.189	1819	1821	1824	rBV2	229	275	0.07%	0.008%
73	12.213	1824	1825	1827	rVB	364	229	0.05%	0.007%
74	12.256	1831	1832	1835	rBV2	414	410	0.10%	0.012%
75	12.323	1838	1843	1851	rVB	227083	287079	68.53%	8.433%
76	12.421	1857	1859	1866	rBV4	561	814	0.19%	0.024%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

77	12.488	1868	1870	1875	rBV	403	584	0.14%	0.017%
78	12.646	1894	1896	1897	rBV	381	218	0.05%	0.006%
79	12.768	1911	1916	1918	rVB2	955	1214	0.29%	0.036%
80	13.006	1952	1955	1957	rBV2	331	313	0.07%	0.009%
81	13.055	1960	1963	1964	rVB2	467	403	0.10%	0.012%
82	13.116	1970	1973	1975	rBV2	352	270	0.06%	0.008%
83	13.164	1980	1981	1983	rBV	414	321	0.08%	0.009%
84	13.225	1989	1991	1993	rBV	271	206	0.05%	0.006%
85	13.329	2004	2008	2009	rBV	252	226	0.05%	0.007%
86	13.890	2098	2100	2103	rVB	260	306	0.07%	0.009%
87	13.920	2103	2105	2106	rBV	287	225	0.05%	0.007%
88	13.963	2110	2112	2115	rVB	383	272	0.06%	0.008%
89	13.987	2115	2116	2119	rBV	264	234	0.06%	0.007%
90	14.061	2127	2128	2131	rBV2	295	243	0.06%	0.007%
91	14.134	2136	2140	2148	rVB2	1398	2172	0.52%	0.064%
92	14.451	2190	2192	2194	rVB	537	352	0.08%	0.010%
93	14.670	2226	2228	2229	rBV	324	197	0.05%	0.006%
94	14.817	2249	2252	2253	rVB	296	277	0.07%	0.008%
95	14.835	2253	2255	2257	rBV2	294	296	0.07%	0.009%
96	14.859	2257	2259	2262	rBV	290	392	0.09%	0.012%
97	15.127	2302	2303	2304	rBV	403	222	0.05%	0.007%
98	15.231	2317	2320	2321	rBV	342	304	0.07%	0.009%
99	16.164	2472	2473	2475	rBV	325	209	0.05%	0.006%
100	16.645	2547	2552	2554	rBV2	393	659	0.16%	0.019%

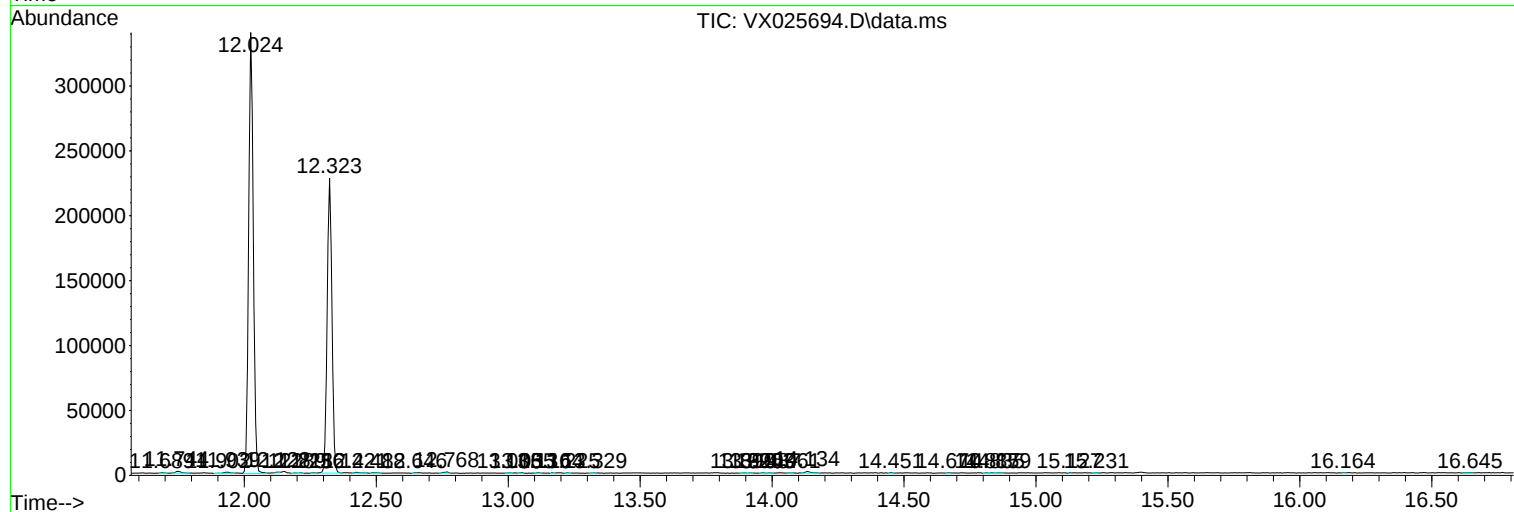
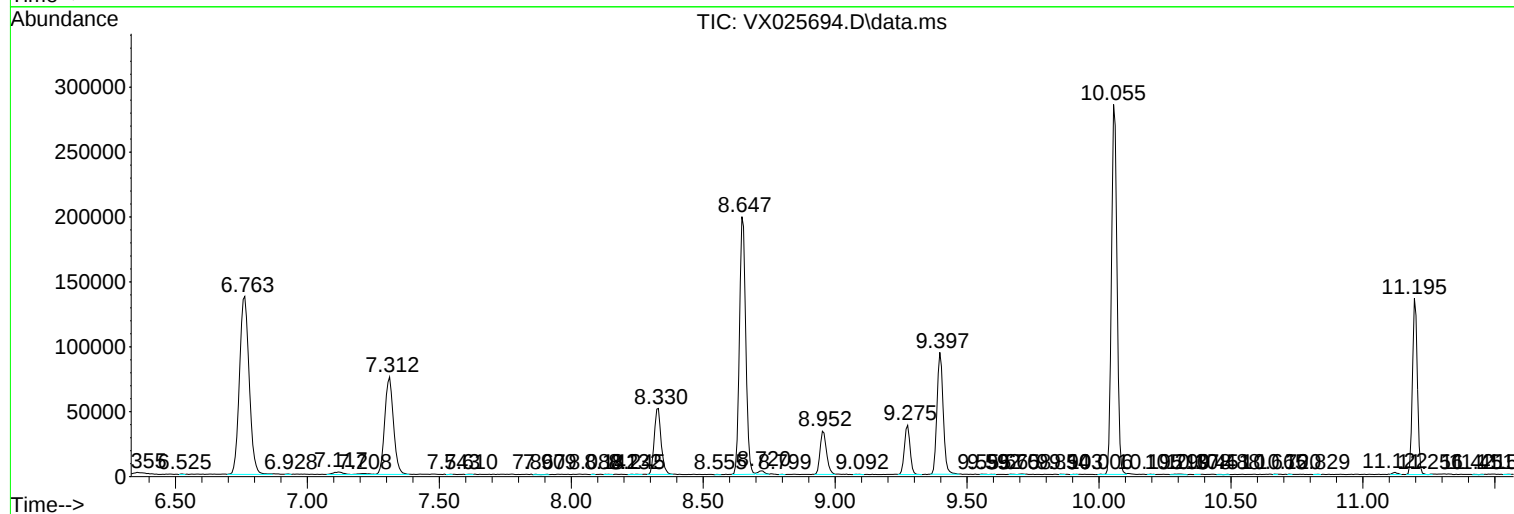
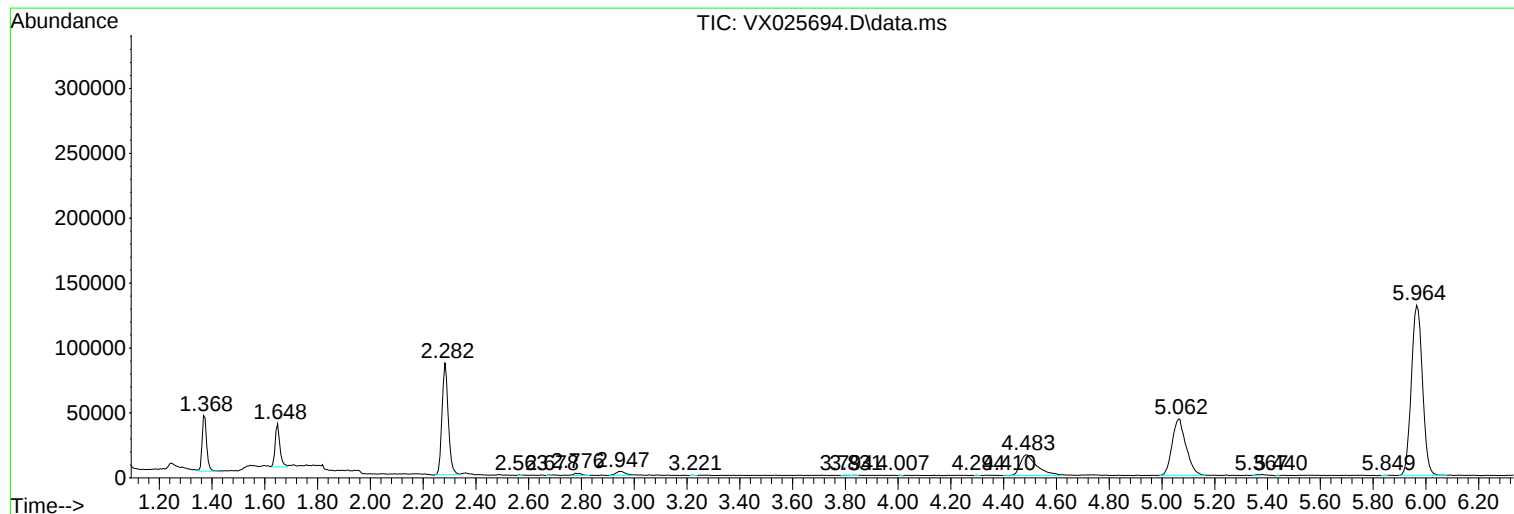
Sum of corrected areas: 3404128

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ALS Vial : 4 Sample Multiplier: 1

Instrument :
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ClientSampleId :
BGKW3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.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\SFAMXML112221WMA.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