

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122821\
 Data File : VX026118.D
 Acq On : 28 Dec 2021 23:28
 Operator : JC/MD
 Sample : M5233-04
 Misc : 8.73g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GBCC2

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: VX026118.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	56	rVB	169502	198495	14.65%	2.089%
2	1.666	91	95	101	rVB	115507	142759	10.54%	1.503%
3	2.294	191	198	205	rBV	336678	521315	38.49%	5.487%
4	2.782	275	278	283	rBV3	1771	2858	0.21%	0.030%
5	2.947	300	305	313	rVB2	5862	12332	0.91%	0.130%
6	3.599	408	412	413	rBV	962	849	0.06%	0.009%
7	3.739	434	435	438	rBV2	615	706	0.05%	0.007%
8	3.934	465	467	469	rVB	659	572	0.04%	0.006%
9	4.270	517	522	524	rBV	594	859	0.06%	0.009%
10	4.361	535	537	539	rBV2	730	592	0.04%	0.006%
11	4.483	548	557	584	rBV	56328	269936	19.93%	2.841%
12	4.916	627	628	631	rBV	457	588	0.04%	0.006%
13	4.977	636	638	641	rVV2	483	683	0.05%	0.007%
14	5.062	641	652	674	rVV2	164838	548828	40.52%	5.776%
15	5.202	674	675	678	rVV2	842	944	0.07%	0.010%
16	5.757	763	766	767	rBV	637	575	0.04%	0.006%
17	5.971	788	801	821	rBV2	474978	1354496	100.00%	14.256%
18	6.147	827	830	833	rBV	618	768	0.06%	0.008%
19	6.227	841	843	846	rVB	536	605	0.04%	0.006%
20	6.361	862	865	866	rBV2	825	800	0.06%	0.008%
21	6.434	874	877	878	rBV2	603	737	0.05%	0.008%
22	6.452	878	880	882	rVV2	830	680	0.05%	0.007%
23	6.537	892	894	897	rBV2	528	618	0.05%	0.007%
24	6.763	921	931	945	rBV	248323	611324	45.13%	6.434%
25	7.111	980	988	996	rBV3	6209	14396	1.06%	0.152%
26	7.208	1001	1004	1008	rBV4	585	821	0.06%	0.009%
27	7.312	1013	1021	1034	rVV	277133	605076	44.67%	6.368%
28	7.464	1044	1046	1047	rBV	901	842	0.06%	0.009%
29	7.799	1098	1101	1103	rVB	578	638	0.05%	0.007%
30	7.940	1122	1124	1125	rBV2	675	573	0.04%	0.006%
31	8.330	1181	1188	1200	rBV	188291	320468	23.66%	3.373%
32	8.482	1208	1213	1214	rBV3	704	991	0.07%	0.010%
33	8.519	1217	1219	1223	rVB2	722	702	0.05%	0.007%
34	8.653	1234	1241	1248	rBV	678782	1067384	78.80%	11.234%
35	8.720	1250	1252	1261	rVB	10116	14605	1.08%	0.154%
36	8.909	1279	1283	1285	rBV3	1231	1934	0.14%	0.020%

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

37	8.952	1285	1290	1300	rVV	121926	199508	14.73%	2.100%
38	9.208	1331	1332	1338	rVV2	433	636	0.05%	0.007%
39	9.275	1340	1343	1344	rBV2	987	1289	0.10%	0.014%
40	9.317	1348	1350	1351	rBV	648	564	0.04%	0.006%
41	9.336	1351	1353	1354	rVV2	892	711	0.05%	0.007%
42	9.409	1357	1365	1379	rVV	307396	597996	44.15%	6.294%
43	9.543	1383	1387	1389	rVB4	1539	1922	0.14%	0.020%
44	9.860	1434	1439	1442	rVB3	572	918	0.07%	0.010%
45	10.061	1464	1472	1485	rBV	460031	725269	53.55%	7.633%
46	10.305	1509	1512	1516	rVV2	1267	1884	0.14%	0.020%
47	10.549	1549	1552	1555	rBV	689	794	0.06%	0.008%
48	10.781	1588	1590	1593	rVB	559	552	0.04%	0.006%
49	10.842	1599	1600	1604	rVB2	655	816	0.06%	0.009%
50	10.927	1613	1614	1616	rBV	699	580	0.04%	0.006%
51	11.067	1634	1637	1638	rVB	596	573	0.04%	0.006%
52	11.085	1638	1640	1642	rBV	487	603	0.04%	0.006%
53	11.122	1642	1646	1652	rVB2	5720	7653	0.57%	0.081%
54	11.201	1653	1659	1668	rVV	444923	594326	43.88%	6.255%
55	11.317	1674	1678	1684	rVB4	3807	7507	0.55%	0.079%
56	11.384	1684	1689	1691	rBV2	767	1097	0.08%	0.012%
57	11.482	1701	1705	1712	rVB3	1753	3967	0.29%	0.042%
58	11.640	1728	1731	1732	rVV3	748	783	0.06%	0.008%
59	11.750	1742	1749	1753	rVV4	3946	6709	0.50%	0.071%
60	11.939	1772	1780	1783	rBV2	2764	4489	0.33%	0.047%
61	11.976	1783	1786	1789	rVB3	1367	1688	0.12%	0.018%
62	12.024	1789	1794	1805	rVB	524860	673346	49.71%	7.087%
63	12.128	1807	1811	1812	rBV2	2399	2664	0.20%	0.028%
64	12.262	1830	1833	1835	rBV	1037	906	0.07%	0.010%
65	12.323	1835	1843	1851	rVV	729837	922269	68.09%	9.707%
66	12.421	1857	1859	1864	rVB3	1565	2367	0.17%	0.025%
67	12.488	1864	1870	1873	rVB4	1300	2406	0.18%	0.025%
68	12.585	1883	1886	1888	rBV	474	646	0.05%	0.007%
69	12.658	1896	1898	1902	rBV3	1143	1496	0.11%	0.016%
70	12.762	1913	1915	1919	rVB3	1109	1477	0.11%	0.016%
71	12.866	1929	1932	1935	rVB2	783	882	0.07%	0.009%
72	13.055	1959	1963	1967	rVB2	890	1312	0.10%	0.014%
73	13.140	1974	1977	1979	rVB	627	719	0.05%	0.008%
74	13.158	1979	1980	1984	rBV	833	879	0.06%	0.009%
75	13.250	1993	1995	2000	rVB	499	760	0.06%	0.008%
76	13.402	2016	2020	2022	rBV2	543	881	0.07%	0.009%

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 Title : VOC Analysis

77	13.500	2033	2036	2037	rVB	922	692	0.05%	0.007%
78	13.591	2046	2051	2055	rBV5	5100	6582	0.49%	0.069%
79	13.683	2064	2066	2071	rBV2	559	586	0.04%	0.006%
80	13.963	2110	2112	2116	rVB2	1226	1708	0.13%	0.018%
81	14.012	2116	2120	2121	rVB2	775	656	0.05%	0.007%
82	14.036	2121	2124	2125	rBV	571	697	0.05%	0.007%
83	14.134	2138	2140	2143	rVV	984	722	0.05%	0.008%
84	14.182	2146	2148	2150	rBV	577	580	0.04%	0.006%
85	14.652	2222	2225	2228	rVB2	700	622	0.05%	0.007%
86	14.823	2251	2253	2256	rVB2	807	857	0.06%	0.009%
87	14.847	2256	2257	2260	rBV	757	988	0.07%	0.010%
88	14.914	2264	2268	2269	rBV3	491	687	0.05%	0.007%
89	15.426	2350	2352	2355	rVB2	851	651	0.05%	0.007%
90	15.469	2357	2359	2361	rBV2	486	554	0.04%	0.006%
91	15.493	2361	2363	2366	rVB2	547	628	0.05%	0.007%
92	15.609	2380	2382	2387	rVB2	773	1070	0.08%	0.011%
93	15.646	2387	2388	2390	rBV	722	619	0.05%	0.007%
94	15.999	2444	2446	2448	rBV	546	710	0.05%	0.007%
95	16.292	2492	2494	2498	rVB	727	918	0.07%	0.010%
96	16.341	2498	2502	2505	rBV2	643	1091	0.08%	0.011%
97	16.639	2549	2551	2553	rVB	891	564	0.04%	0.006%
98	16.664	2553	2555	2560	rVB2	505	701	0.05%	0.007%
99	16.700	2560	2561	2564	rBV2	593	553	0.04%	0.006%
100	16.773	2571	2573	2575	rBV2	572	557	0.04%	0.006%

Sum of corrected areas: 9501186

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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