

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039306.D
 Acq On : 18 Dec 2023 13:08
 Operator : JC/MD
 Sample : 05806-09ME
 Misc : 4.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E0LQ9ME

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: VX039306.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	26	29	35	rVB2	2534	3041	0.39%	0.047%
2	1.368	43	46	61	rVB	49230	81956	10.53%	1.267%
3	1.648	89	92	107	rBV	18200	40588	5.21%	0.628%
4	2.276	189	195	207	rBV	128487	215001	27.62%	3.325%
5	2.776	274	277	286	rVB3	2799	5578	0.72%	0.086%
6	2.946	298	305	315	rBV	6416	16149	2.07%	0.250%
7	3.142	335	337	340	rBV2	255	244	0.03%	0.004%
8	3.227	349	351	358	rVB2	283	485	0.06%	0.008%
9	3.666	421	423	427	rBV2	332	382	0.05%	0.006%
10	3.696	427	428	431	rVV	265	273	0.04%	0.004%
11	3.751	433	437	438	rVB2	290	328	0.04%	0.005%
12	3.971	469	473	476	rBV2	250	401	0.05%	0.006%
13	4.099	493	494	497	rBV2	385	437	0.06%	0.007%
14	4.190	505	509	510	rBV2	183	219	0.03%	0.003%
15	4.489	547	558	588	rBV2	49592	222884	28.63%	3.447%
16	5.062	639	652	666	rBV	94251	303932	39.04%	4.700%
17	5.172	669	670	673	rVB2	432	313	0.04%	0.005%
18	5.202	673	675	678	rBV3	312	351	0.05%	0.005%
19	5.403	704	708	712	rVB4	571	953	0.12%	0.015%
20	5.537	727	730	733	rBV2	503	818	0.11%	0.013%
21	5.964	789	800	819	rBV2	272533	778533	100.00%	12.040%
22	6.153	829	831	833	rVB3	308	270	0.03%	0.004%
23	6.190	834	837	839	rVB2	325	380	0.05%	0.006%
24	6.226	839	843	844	rBV2	307	311	0.04%	0.005%
25	6.367	861	866	867	rBV3	1111	1467	0.19%	0.023%
26	6.501	886	888	891	rVB	317	251	0.03%	0.004%
27	6.550	893	896	897	rBV2	317	346	0.04%	0.005%
28	6.568	897	899	901	rVB2	257	219	0.03%	0.003%
29	6.763	921	931	950	rBV	243301	610005	78.35%	9.434%
30	7.116	983	989	990	rBV4	2252	3457	0.44%	0.053%
31	7.214	1000	1005	1012	rBV3	3020	6116	0.79%	0.095%
32	7.305	1012	1020	1034	rVB	155106	355310	45.64%	5.495%
33	7.488	1048	1050	1053	rVB2	434	417	0.05%	0.006%
34	7.757	1091	1094	1096	rBV2	307	416	0.05%	0.006%
35	7.866	1108	1112	1114	rVB2	239	312	0.04%	0.005%
36	7.970	1124	1129	1138	rVB5	918	2386	0.31%	0.037%

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

37	8.092	1143	1149	1153	rVB3	331	523	0.07%	0.008%
38	8.238	1172	1173	1178	rBV2	275	444	0.06%	0.007%
39	8.324	1181	1187	1197	rBV	100001	174452	22.41%	2.698%
40	8.513	1213	1218	1223	rVB4	599	1059	0.14%	0.016%
41	8.580	1227	1229	1234	rBV2	290	335	0.04%	0.005%
42	8.647	1234	1240	1254	rBV	355245	592832	76.15%	9.168%
43	8.952	1285	1290	1302	rVV	71714	113999	14.64%	1.763%
44	9.110	1314	1316	1321	rVB5	921	1307	0.17%	0.020%
45	9.153	1321	1323	1326	rVV2	275	269	0.03%	0.004%
46	9.275	1338	1343	1356	rBV	11622	17710	2.27%	0.274%
47	9.397	1357	1363	1380	rBV	266768	485566	62.37%	7.509%
48	9.610	1395	1398	1401	rVB4	447	574	0.07%	0.009%
49	9.671	1405	1408	1412	rVV3	454	547	0.07%	0.008%
50	9.714	1412	1415	1422	rVB5	1010	1688	0.22%	0.026%
51	9.909	1443	1447	1448	rBV	202	249	0.03%	0.004%
52	10.055	1465	1471	1486	rBV	511708	714952	91.83%	11.057%
53	10.299	1507	1511	1512	rBV	250	327	0.04%	0.005%
54	10.311	1512	1513	1516	rVB2	321	271	0.03%	0.004%
55	10.787	1589	1591	1595	rVB2	349	383	0.05%	0.006%
56	10.823	1595	1597	1601	rVB2	292	349	0.04%	0.005%
57	11.091	1638	1641	1645	rBV3	605	867	0.11%	0.013%
58	11.195	1652	1658	1667	rBV	304432	390885	50.21%	6.045%
59	11.311	1674	1677	1679	rBV2	249	297	0.04%	0.005%
60	11.451	1698	1700	1703	rVV2	318	416	0.05%	0.006%
61	11.475	1703	1704	1708	rVV2	362	485	0.06%	0.008%
62	11.549	1714	1716	1719	rBV2	359	260	0.03%	0.004%
63	11.585	1719	1722	1725	rVB2	293	297	0.04%	0.005%
64	11.634	1727	1730	1735	rVB3	792	924	0.12%	0.014%
65	11.683	1735	1738	1739	rBV	660	536	0.07%	0.008%
66	11.707	1740	1742	1747	rVV3	650	948	0.12%	0.015%
67	11.756	1747	1750	1751	rVV	254	256	0.03%	0.004%
68	11.847	1762	1765	1768	rVV2	222	261	0.03%	0.004%
69	11.975	1784	1786	1789	rVB2	335	349	0.04%	0.005%
70	12.024	1789	1794	1805	rBV	561229	701963	90.16%	10.856%
71	12.231	1826	1828	1831	rBV3	603	615	0.08%	0.010%
72	12.323	1837	1843	1853	rBV	418918	546028	70.14%	8.444%
73	12.585	1880	1886	1887	rBV2	436	661	0.08%	0.010%
74	12.683	1899	1902	1903	rBV2	289	247	0.03%	0.004%
75	12.762	1910	1915	1916	rBV2	919	868	0.11%	0.013%
76	12.878	1932	1934	1935	rBV2	427	291	0.04%	0.005%

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77	12.945	1943	1945	1948	rBV2	285	288	0.04%	0.004%
78	12.975	1948	1950	1954	rVB2	524	562	0.07%	0.009%
79	13.042	1957	1961	1963	rBV2	448	546	0.07%	0.008%
80	13.268	1994	1998	2003	rVV3	3061	4369	0.56%	0.068%
81	13.384	2014	2017	2021	rBV2	3516	4239	0.54%	0.066%
82	13.591	2046	2051	2056	rVB5	949	1284	0.16%	0.020%
83	13.682	2062	2066	2067	rBV2	601	816	0.10%	0.013%
84	13.701	2067	2069	2072	rVV3	1051	1108	0.14%	0.017%
85	13.847	2089	2093	2097	rVB3	2424	3158	0.41%	0.049%
86	13.969	2110	2113	2115	rBV2	511	572	0.07%	0.009%
87	14.042	2121	2125	2129	rBV	8648	9705	1.25%	0.150%
88	14.103	2133	2135	2137	rVV3	860	712	0.09%	0.011%
89	14.134	2137	2140	2145	rVB4	1691	1999	0.26%	0.031%
90	14.188	2147	2149	2152	rBV2	887	616	0.08%	0.010%
91	14.298	2166	2167	2171	rBV3	320	369	0.05%	0.006%
92	14.408	2181	2185	2187	rBV3	880	1505	0.19%	0.023%
93	14.469	2193	2195	2198	rBV4	794	728	0.09%	0.011%
94	14.615	2216	2219	2225	rVB2	2537	3103	0.40%	0.048%
95	14.755	2239	2242	2247	rBV	8906	10745	1.38%	0.166%
96	15.213	2314	2317	2325	rVB7	2311	3596	0.46%	0.056%
97	15.493	2359	2363	2369	rVB3	3618	5036	0.65%	0.078%
98	15.609	2380	2382	2383	rBV2	628	387	0.05%	0.006%
99	16.218	2481	2482	2485	rBV2	546	579	0.07%	0.009%
100	16.755	2568	2570	2572	rBV2	421	302	0.04%	0.005%

Sum of corrected areas: 6466143

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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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MSVOA_X
ClientSampleId :
E0LQ9ME

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

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