

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046159.D
 Acq On : 07 Dec 2021 22:55
 Operator : SY/MD
 Sample : M4960-05 10X
 Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 43 Sample Multiplier: 1

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_U\Method\SFAMULM112921WMA.M

Title : VOC Analysis

Signal : TIC: VU046169.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	95	rVB	119483	132295	15.11%	1.843%
2	1.919	171	180	193	rBV	81478	104209	11.90%	1.451%
3	2.571	371	383	425	rVB	192222	321832	36.77%	4.483%
4	2.800	449	454	462	rVB2	261	337	0.04%	0.005%
5	3.051	525	532	540	rVB3	1229	1976	0.23%	0.028%
6	3.189	560	575	595	rVB	11159	26212	2.99%	0.365%
7	3.436	649	652	656	rBV	177	189	0.02%	0.003%
8	3.520	675	678	681	rBV	154	158	0.02%	0.002%
9	3.571	691	694	697	rBV	187	157	0.02%	0.002%
10	3.661	720	722	726	rBV	144	139	0.02%	0.002%
11	3.915	795	801	805	rBB	139	213	0.02%	0.003%
12	3.989	820	824	828	rBV	124	155	0.02%	0.002%
13	4.231	890	899	901	rBV	165	299	0.03%	0.004%
14	4.269	909	911	915	rBV	129	135	0.02%	0.002%
15	4.327	926	929	935	rBB	185	213	0.02%	0.003%
16	4.362	937	940	944	rBB	150	146	0.02%	0.002%
17	4.639	1009	1026	1068	rBV	76144	230782	26.36%	3.214%
18	4.931	1112	1117	1120	rBB2	318	351	0.04%	0.005%
19	4.957	1121	1125	1128	rBV	135	135	0.02%	0.002%
20	5.067	1143	1159	1184	rVB	146224	333355	38.08%	4.643%
21	5.295	1227	1230	1232	rBV	242	153	0.02%	0.002%
22	5.359	1248	1250	1254	rBV2	362	237	0.03%	0.003%
23	5.375	1254	1255	1263	rVB	227	211	0.02%	0.003%
24	5.423	1268	1270	1274	rBV	134	144	0.02%	0.002%
25	5.494	1289	1292	1296	rBV	133	163	0.02%	0.002%
26	5.578	1314	1318	1320	rBV	142	149	0.02%	0.002%
27	5.594	1320	1323	1328	rVB	510	333	0.04%	0.005%
28	5.729	1343	1365	1391	rBV2	324332	875348	100.00%	12.192%
29	5.967	1435	1439	1440	rBV2	484	295	0.03%	0.004%
30	6.038	1458	1461	1462	rBV	265	153	0.02%	0.002%
31	6.111	1481	1484	1487	rBV2	265	217	0.02%	0.003%
32	6.250	1513	1527	1550	rBV	291306	550902	62.94%	7.673%
33	6.533	1605	1615	1629	rBV3	4352	8976	1.03%	0.125%
34	6.693	1649	1665	1683	rBV	195873	377214	43.09%	5.254%
35	6.928	1735	1738	1740	rBV	163	131	0.01%	0.002%
36	7.041	1767	1773	1781	rBB2	414	707	0.08%	0.010%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046159.D
 Acq On : 07 Dec 2021 22:55
 Operator : SY/MD
 Sample : M4960-05 10X
 Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 43 Sample Multiplier: 1

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_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.083	1782	1786	1789	rBV	167	196	0.02%	0.003%
38	7.144	1802	1805	1808	rBB	161	127	0.01%	0.002%
39	7.484	1908	1911	1914	rBV	181	178	0.02%	0.002%
40	7.568	1924	1937	1951	rBV	110198	191567	21.88%	2.668%
41	7.732	1984	1988	1997	rBV	206	340	0.04%	0.005%
42	7.783	1998	2004	2011	rBV3	731	1249	0.14%	0.017%
43	7.899	2025	2040	2056	rBV	428518	735982	84.08%	10.251%
44	8.179	2116	2127	2147	rBV	75813	126779	14.48%	1.766%
45	8.436	2205	2207	2211	rBV	166	159	0.02%	0.002%
46	8.478	2217	2220	2224	rVB2	169	146	0.02%	0.002%
47	8.545	2236	2241	2244	rBV	142	191	0.02%	0.003%
48	8.636	2256	2269	2295	rBV	256354	456956	52.20%	6.365%
49	8.861	2334	2339	2345	rBV2	496	726	0.08%	0.010%
50	8.915	2349	2356	2359	rBV2	1948	2445	0.28%	0.034%
51	8.970	2370	2373	2376	rBV	292	143	0.02%	0.002%
52	9.115	2415	2418	2420	rBV	178	134	0.02%	0.002%
53	9.163	2429	2433	2436	rBV4	759	651	0.07%	0.009%
54	9.208	2445	2447	2449	rBV2	252	130	0.01%	0.002%
55	9.333	2482	2486	2488	rBV	628	559	0.06%	0.008%
56	9.417	2499	2512	2536	rBV	412567	685818	78.35%	9.552%
57	9.571	2553	2560	2567	rBV	579	807	0.09%	0.011%
58	9.697	2592	2599	2600	rBV3	810	928	0.11%	0.013%
59	10.025	2693	2701	2713	rBV5	1292	2848	0.33%	0.040%
60	10.076	2713	2717	2720	rVV2	232	190	0.02%	0.003%
61	10.115	2725	2729	2736	rVB3	751	960	0.11%	0.013%
62	10.243	2763	2769	2782	rVB7	1452	3323	0.38%	0.046%
63	10.359	2796	2805	2810	rBV4	2687	4227	0.48%	0.059%
64	10.481	2840	2843	2845	rBV2	228	177	0.02%	0.002%
65	10.558	2861	2867	2868	rBV	964	852	0.10%	0.012%
66	10.623	2882	2887	2895	rBV5	1368	1581	0.18%	0.022%
67	10.671	2895	2902	2914	rVB4	3530	5071	0.58%	0.071%
68	10.758	2916	2929	2941	rBV	284877	454779	51.95%	6.334%
69	10.889	2959	2970	2971	rBV5	823	1289	0.15%	0.018%
70	10.954	2984	2990	2993	rBV3	441	467	0.05%	0.007%
71	11.005	3003	3006	3008	rBV3	731	450	0.05%	0.006%
72	11.063	3017	3024	3031	rBV3	999	1592	0.18%	0.022%
73	11.208	3064	3069	3074	rVB3	689	716	0.08%	0.010%
74	11.282	3087	3092	3096	rBV3	392	489	0.06%	0.007%
75	11.311	3096	3101	3109	rVV5	1761	2496	0.29%	0.035%
76	11.375	3114	3121	3125	rBV4	1840	2465	0.28%	0.034%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046159.D
 Acq On : 07 Dec 2021 22:55
 Operator : SY/MD
 Sample : M4960-05 10X
 Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 43 Sample Multiplier: 1

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_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

77	11.417	3129	3134	3140	rVB4	3683	4335	0.50%	0.060%
78	11.578	3176	3184	3191	rBV5	1942	3335	0.38%	0.046%
79	11.696	3213	3221	3230	rBV8	3999	6628	0.76%	0.092%
80	11.812	3245	3257	3271	rBV	491130	753657	86.10%	10.497%
81	11.896	3281	3283	3285	rVB	291	139	0.02%	0.002%
82	11.944	3287	3298	3301	rBV4	3019	4666	0.53%	0.065%
83	12.037	3323	3327	3332	rVB3	511	430	0.05%	0.006%
84	12.076	3332	3339	3344	rBV5	592	795	0.09%	0.011%
85	12.195	3360	3376	3390	rBV	443119	715015	81.68%	9.959%
86	12.323	3409	3416	3418	rBV4	2179	2445	0.28%	0.034%
87	12.388	3428	3436	3438	rBV3	1578	2045	0.23%	0.028%
88	12.725	3538	3541	3543	rBV2	684	495	0.06%	0.007%
89	13.024	3628	3634	3639	rBV4	649	867	0.10%	0.012%
90	13.060	3641	3645	3647	rVV2	451	299	0.03%	0.004%
91	13.587	3803	3809	3818	rVB5	2285	3017	0.34%	0.042%
92	14.085	3957	3964	3973	rVB2	7702	10728	1.23%	0.149%
93	14.192	3989	3997	4008	rBV4	2395	3680	0.42%	0.051%
94	14.272	4017	4022	4031	rBV4	566	744	0.08%	0.010%
95	14.520	4097	4099	4100	rBV4	429	185	0.02%	0.003%
96	14.574	4109	4116	4124	rBV4	1658	2860	0.33%	0.040%
97	14.745	4167	4169	4175	rBV2	321	308	0.04%	0.004%
98	14.799	4183	4186	4187	rBV3	396	245	0.03%	0.003%
99	14.973	4237	4240	4242	rBV2	420	290	0.03%	0.004%
100	15.214	4307	4315	4321	rBV9	2260	3638	0.42%	0.051%

Sum of corrected areas: 7179650

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046159.D
Acq On : 07 Dec 2021 22:55
Operator : SY/MD
Sample : M4960-05 10X
Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046159.D
Acq On : 07 Dec 2021 22:55
Operator : SY/MD
Sample : M4960-05 10X
Misc : 6.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 43 Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
