

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071124\
 Data File : VU059908.D
 Acq On : 11 Jul 2024 15:21
 Operator : MD/SY
 Sample : P3177-16ME
 Misc : 5.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4BY2ME

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\SFAMULM070224WMA.M
 Title : VOC Analysis

Signal : TIC: VU059908.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.486	55	61	65	rBV3	1661	1845	0.27%	0.033%
2	1.595	87	95	118	rBV	48880	79596	11.81%	1.443%
3	1.862	143	178	181	rBV4	36208	113511	16.85%	2.058%
4	1.891	182	187	198	rVV	38463	64106	9.51%	1.163%
5	2.547	378	391	409	rBV	114678	187453	27.82%	3.399%
6	2.634	411	418	436	rVB4	2025	4518	0.67%	0.082%
7	2.772	455	461	472	rBV3	739	1331	0.20%	0.024%
8	2.949	503	516	534	rBV	12423	26819	3.98%	0.486%
9	3.029	535	541	554	rVB6	2716	5566	0.83%	0.101%
10	3.177	573	587	604	rBV2	7475	19784	2.94%	0.359%
11	3.303	623	626	633	rVB2	203	227	0.03%	0.004%
12	3.364	641	645	651	rVV	269	248	0.04%	0.004%
13	3.402	652	657	661	rVB2	218	232	0.03%	0.004%
14	3.444	666	670	675	rBV2	264	269	0.04%	0.005%
15	3.547	699	702	706	rBV2	151	148	0.02%	0.003%
16	3.573	707	710	713	rVV	210	153	0.02%	0.003%
17	3.660	733	737	740	rBV2	278	223	0.03%	0.004%
18	4.062	858	862	868	rVB2	259	230	0.03%	0.004%
19	4.110	868	877	882	rBV2	272	378	0.06%	0.007%
20	4.139	882	886	888	rBV	347	158	0.02%	0.003%
21	4.184	892	900	908	rVB2	328	562	0.08%	0.010%
22	4.332	943	946	951	rVB	222	205	0.03%	0.004%
23	4.361	951	955	959	rBV2	204	216	0.03%	0.004%
24	4.573	1017	1021	1027	rVB	229	250	0.04%	0.005%
25	4.627	1027	1038	1077	rBV	49448	155240	23.04%	2.815%
26	5.052	1155	1170	1192	rBV	114576	253791	37.67%	4.602%
27	5.319	1250	1253	1255	rVV2	283	193	0.03%	0.003%
28	5.335	1255	1258	1263	rVV2	136	143	0.02%	0.003%
29	5.402	1275	1279	1282	rBV2	231	157	0.02%	0.003%
30	5.714	1357	1376	1407	rBV2	239460	640099	95.01%	11.608%
31	5.955	1448	1451	1454	rVB	272	179	0.03%	0.003%
32	6.007	1464	1467	1470	rBV	396	237	0.04%	0.004%
33	6.094	1491	1494	1498	rVB2	256	188	0.03%	0.003%
34	6.123	1498	1503	1507	rBV2	235	273	0.04%	0.005%
35	6.238	1524	1539	1560	rBV	259107	506535	75.18%	9.186%
36	6.460	1605	1608	1611	rBV3	370	215	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
 Title : VOC Analysis

37	6.521	1621	1627	1640	rBV5	1520	2835	0.42%	0.051%
38	6.602	1646	1652	1655	rVB	576	512	0.08%	0.009%
39	6.682	1664	1677	1699	rBV	146410	290925	43.18%	5.276%
40	6.814	1714	1718	1721	rVV2	267	194	0.03%	0.004%
41	7.081	1796	1801	1803	rBV	198	173	0.03%	0.003%
42	7.119	1808	1813	1818	rBV2	135	185	0.03%	0.003%
43	7.200	1832	1838	1840	rBV3	809	702	0.10%	0.013%
44	7.296	1865	1868	1870	rVV	222	155	0.02%	0.003%
45	7.335	1877	1880	1885	rBV2	159	151	0.02%	0.003%
46	7.463	1917	1920	1927	rVB2	273	220	0.03%	0.004%
47	7.560	1938	1950	1969	rBV2	73640	134012	19.89%	2.430%
48	7.663	1978	1982	1989	rVB2	447	568	0.08%	0.010%
49	7.708	1989	1996	1998	rBV2	360	383	0.06%	0.007%
50	7.733	2002	2004	2008	rVB	452	223	0.03%	0.004%
51	7.814	2026	2029	2031	rBV2	213	147	0.02%	0.003%
52	7.891	2040	2053	2073	rBV	273228	479794	71.21%	8.701%
53	8.029	2094	2096	2102	rBV3	262	218	0.03%	0.004%
54	8.177	2128	2142	2160	rBV2	50555	91559	13.59%	1.660%
55	8.296	2177	2179	2188	rVB2	239	306	0.05%	0.006%
56	8.341	2188	2193	2197	rBV2	356	327	0.05%	0.006%
57	8.463	2222	2231	2237	rBV3	1041	1559	0.23%	0.028%
58	8.547	2255	2257	2262	rVB2	261	146	0.02%	0.003%
59	8.582	2265	2268	2273	rVB2	207	211	0.03%	0.004%
60	8.643	2273	2287	2325	rBV	122437	318792	47.32%	5.781%
61	8.775	2326	2328	2331	rBV3	385	268	0.04%	0.005%
62	8.930	2372	2376	2382	rVB3	434	427	0.06%	0.008%
63	8.978	2388	2391	2395	rBV	255	209	0.03%	0.004%
64	9.122	2430	2436	2441	rBV	269	397	0.06%	0.007%
65	9.219	2460	2466	2468	rBV2	184	179	0.03%	0.003%
66	9.412	2512	2526	2557	rBV	388715	673742	100.00%	12.218%
67	9.605	2579	2586	2593	rVB2	868	1215	0.18%	0.022%
68	9.695	2608	2614	2616	rBV3	514	434	0.06%	0.008%
69	9.737	2622	2627	2630	rBV	180	204	0.03%	0.004%
70	9.843	2656	2660	2664	rBV	221	228	0.03%	0.004%
71	10.756	2929	2944	2967	rBV	229523	394132	58.50%	7.147%
72	10.884	2978	2984	2992	rVB3	824	1287	0.19%	0.023%
73	11.129	3057	3060	3065	rBV2	160	151	0.02%	0.003%
74	11.196	3078	3081	3084	rBV	219	151	0.02%	0.003%
75	11.312	3110	3117	3121	rBV	285	373	0.06%	0.007%
76	11.392	3138	3142	3146	rBV	248	242	0.04%	0.004%

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77	11.547	3187	3190	3194	rVB2	267	181	0.03%	0.003%
78	11.704	3234	3239	3243	rBV2	357	364	0.05%	0.007%
79	11.807	3259	3271	3294	rBV	360977	595740	88.42%	10.803%
80	11.984	3320	3326	3328	rBV3	443	410	0.06%	0.007%
81	12.007	3328	3333	3337	rVV3	295	300	0.04%	0.005%
82	12.190	3375	3390	3412	rBV	273176	447758	66.46%	8.120%
83	12.370	3442	3446	3452	rBV	320	277	0.04%	0.005%
84	12.531	3492	3496	3499	rBV	420	356	0.05%	0.006%
85	12.920	3612	3617	3619	rBV2	1032	817	0.12%	0.015%
86	13.380	3756	3760	3764	rBV	282	315	0.05%	0.006%
87	13.495	3793	3796	3799	rBV2	236	167	0.02%	0.003%
88	13.544	3807	3811	3816	rBV2	358	371	0.06%	0.007%
89	13.637	3838	3840	3844	rVB3	469	303	0.04%	0.005%
90	13.807	3891	3893	3898	rBV3	312	231	0.03%	0.004%
91	13.871	3907	3913	3917	rBV2	285	371	0.06%	0.007%
92	14.441	4088	4090	4092	rBV	259	174	0.03%	0.003%
93	14.566	4124	4129	4131	rBV2	569	532	0.08%	0.010%
94	14.691	4166	4168	4172	rBV3	307	240	0.04%	0.004%
95	14.849	4214	4217	4219	rBV	387	269	0.04%	0.005%
96	14.939	4242	4245	4247	rBV	362	215	0.03%	0.004%
97	14.978	4254	4257	4261	rVB2	783	591	0.09%	0.011%
98	15.543	4431	4433	4435	rBV	427	160	0.02%	0.003%
99	15.659	4466	4469	4472	rBV2	599	375	0.06%	0.007%
100	16.569	4749	4752	4754	rBV	867	612	0.09%	0.011%

Sum of corrected areas: 5514343

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Instrument :
MSVOA_U
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A4BY2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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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Instrument :
MSVOA_U
ClientSampleId :
A4BY2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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