

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU122018\
 Data File : VU028833.D
 Acq On : 20 Dec 2018 18:42
 Operator : MD/SY
 Sample : J6419-14ME
 Misc : 5.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BF042ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.395	62	69	84	rVB	92440	104300	7.71%	1.386%
2	1.640	141	145	155	rVB	63003	63531	4.70%	0.844%
3	2.235	319	330	344	rBV	152922	233516	17.26%	3.104%
4	2.331	357	360	361	rBV	733	400	0.03%	0.005%
5	2.630	446	453	460	rBV3	1310	2521	0.19%	0.034%
6	2.682	463	469	481	rVB3	1940	3410	0.25%	0.045%
7	2.829	504	515	531	rVB	4308	9405	0.70%	0.125%
8	2.916	540	542	545	rVB	280	141	0.01%	0.002%
9	3.190	624	627	630	rBV	357	256	0.02%	0.003%
10	3.312	661	665	671	rVB	79	89	0.01%	0.001%
11	3.540	733	736	737	rBV	171	79	0.01%	0.001%
12	3.659	770	773	778	rVB	93	85	0.01%	0.001%
13	3.736	793	797	801	rVB	140	107	0.01%	0.001%
14	3.778	806	810	813	rBV	86	77	0.01%	0.001%
15	3.820	817	823	827	rBV	99	90	0.01%	0.001%
16	3.858	831	835	839	rVV2	234	152	0.01%	0.002%
17	3.961	865	867	870	rVB	201	76	0.01%	0.001%
18	4.138	918	922	925	rVB	107	74	0.01%	0.001%
19	4.193	925	939	982	rBV	47858	176368	13.03%	2.344%
20	4.521	1039	1041	1045	rVB	208	97	0.01%	0.001%
21	4.559	1045	1053	1054	rBV	257	283	0.02%	0.004%
22	4.643	1061	1079	1110	rVB	110288	265134	19.60%	3.524%
23	4.752	1110	1113	1116	rBV	118	89	0.01%	0.001%
24	4.794	1123	1126	1132	rVB	111	98	0.01%	0.001%
25	4.826	1132	1136	1141	rBV	96	103	0.01%	0.001%
26	4.881	1150	1153	1157	rBV3	376	354	0.03%	0.005%
27	4.929	1165	1168	1173	rVB2	265	206	0.02%	0.003%
28	4.955	1173	1176	1179	rBV	122	101	0.01%	0.001%
29	4.971	1179	1181	1185	rVV2	144	126	0.01%	0.002%
30	5.009	1189	1193	1195	rBV	97	79	0.01%	0.001%
31	5.032	1198	1200	1205	rVB	88	75	0.01%	0.001%
32	5.148	1231	1236	1237	rBV	132	81	0.01%	0.001%
33	5.196	1246	1251	1255	rBV2	175	162	0.01%	0.002%
34	5.241	1261	1265	1267	rBV	109	89	0.01%	0.001%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU122018\
 Data File : VU028833.D
 Acq On : 20 Dec 2018 18:42
 Operator : MD/SY
 Sample : J6419-14ME
 Misc : 5.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BF042ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
 Title : VOC Analysis

35	5.328	1270	1292	1324	rBV2	254132	707594	52.30%	9.405%
36	5.517	1349	1351	1353	rVB	340	133	0.01%	0.002%
37	5.614	1374	1381	1383	rBV3	937	1122	0.08%	0.015%
38	5.768	1426	1429	1435	rBV	89	87	0.01%	0.001%
39	5.881	1449	1464	1489	rBV	279497	578132	42.73%	7.684%
40	6.128	1536	1541	1543	rBV	195	150	0.01%	0.002%
41	6.180	1549	1557	1568	rVB5	2009	3360	0.25%	0.045%
42	6.251	1571	1579	1581	rBV4	1339	1683	0.12%	0.022%
43	6.328	1588	1603	1626	rBV	158036	326168	24.11%	4.335%
44	6.456	1638	1643	1646	rBV2	350	306	0.02%	0.004%
45	6.482	1648	1651	1654	rVB	133	85	0.01%	0.001%
46	6.575	1677	1680	1683	rBV	94	79	0.01%	0.001%
47	6.665	1702	1708	1711	rBV	161	143	0.01%	0.002%
48	6.787	1742	1746	1749	rBV	202	139	0.01%	0.002%
49	6.881	1769	1775	1779	rBV3	405	505	0.04%	0.007%
50	6.977	1802	1805	1814	rVB	105	102	0.01%	0.001%
51	7.170	1858	1865	1868	rBV	81	101	0.01%	0.001%
52	7.225	1870	1882	1910	rVB	86739	165551	12.24%	2.200%
53	7.386	1928	1932	1936	rBV	162	134	0.01%	0.002%
54	7.440	1941	1949	1952	rBV	239	213	0.02%	0.003%
55	7.472	1955	1959	1960	rBV	523	311	0.02%	0.004%
56	7.562	1974	1987	2005	rBV	310957	567406	41.94%	7.542%
57	7.807	2059	2063	2065	rBV	330	156	0.01%	0.002%
58	7.852	2066	2077	2098	rBV2	58528	111368	8.23%	1.480%
59	8.009	2124	2126	2130	rVB	149	87	0.01%	0.001%
60	8.038	2132	2135	2137	rVB	226	139	0.01%	0.002%
61	8.173	2169	2177	2179	rBV2	224	306	0.02%	0.004%
62	8.225	2179	2193	2211	rVV	789825	1353053	100.00%	17.984%
63	8.321	2213	2223	2249	rVB	232960	447962	33.11%	5.954%
64	8.549	2292	2294	2296	rBV	223	102	0.01%	0.001%
65	8.607	2310	2312	2313	rBV	264	109	0.01%	0.001%
66	8.640	2313	2322	2328	rVV3	1125	2049	0.15%	0.027%
67	8.668	2329	2331	2334	rVB	203	85	0.01%	0.001%
68	8.694	2338	2339	2342	rVB	287	131	0.01%	0.002%
69	8.713	2342	2345	2350	rBV2	180	154	0.01%	0.002%
70	8.787	2365	2368	2371	rVB	200	113	0.01%	0.002%
71	8.877	2393	2396	2399	rVB2	308	175	0.01%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU122018\
 Data File : VU028833.D
 Acq On : 20 Dec 2018 18:42
 Operator : MD/SY
 Sample : J6419-14ME
 Misc : 5.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BF042ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
 Title : VOC Analysis

72	8.916	2401	2408	2411	rBV	143	177	0.01%	0.002%
73	8.939	2411	2415	2418	rBV	105	103	0.01%	0.001%
74	9.090	2449	2462	2498	rBV	411571	724619	53.55%	9.631%
75	9.318	2531	2533	2538	rBV	169	111	0.01%	0.001%
76	9.379	2543	2552	2566	rBV3	3456	5482	0.41%	0.073%
77	9.784	2671	2678	2683	rBV4	1053	1287	0.10%	0.017%
78	9.964	2732	2734	2737	rBV	168	130	0.01%	0.002%
79	10.016	2748	2750	2753	rVB	238	92	0.01%	0.001%
80	10.086	2768	2772	2774	rBV	159	102	0.01%	0.001%
81	10.434	2868	2880	2902	rBV	255890	409077	30.23%	5.437%
82	10.684	2952	2958	2962	rBV3	505	549	0.04%	0.007%
83	10.758	2979	2981	2983	rBV	171	74	0.01%	0.001%
84	10.774	2983	2986	2988	rBV2	231	165	0.01%	0.002%
85	10.864	3011	3014	3017	rBV	141	103	0.01%	0.001%
86	10.884	3017	3020	3022	rVV2	306	181	0.01%	0.002%
87	10.922	3029	3032	3033	rBV2	230	139	0.01%	0.002%
88	11.086	3081	3083	3086	rVB	296	104	0.01%	0.001%
89	11.279	3141	3143	3149	rVB	234	133	0.01%	0.002%
90	11.356	3164	3167	3168	rBV	197	89	0.01%	0.001%
91	11.427	3186	3189	3192	rBV	225	161	0.01%	0.002%
92	11.485	3195	3207	3229	rBV	446917	703634	52.00%	9.352%
93	11.861	3311	3324	3341	rBV	330879	542008	40.06%	7.204%
94	12.051	3381	3383	3386	rVB2	428	257	0.02%	0.003%
95	12.067	3386	3388	3392	rBV2	447	211	0.02%	0.003%
96	12.106	3399	3400	3403	rBV2	257	165	0.01%	0.002%
97	12.180	3418	3423	3424	rBV2	286	274	0.02%	0.004%
98	12.434	3498	3502	3506	rVB3	373	288	0.02%	0.004%
99	12.482	3507	3517	3526	rVV4	1236	2614	0.19%	0.035%
100	12.797	3613	3615	3616	rBV4	229	90	0.01%	0.001%

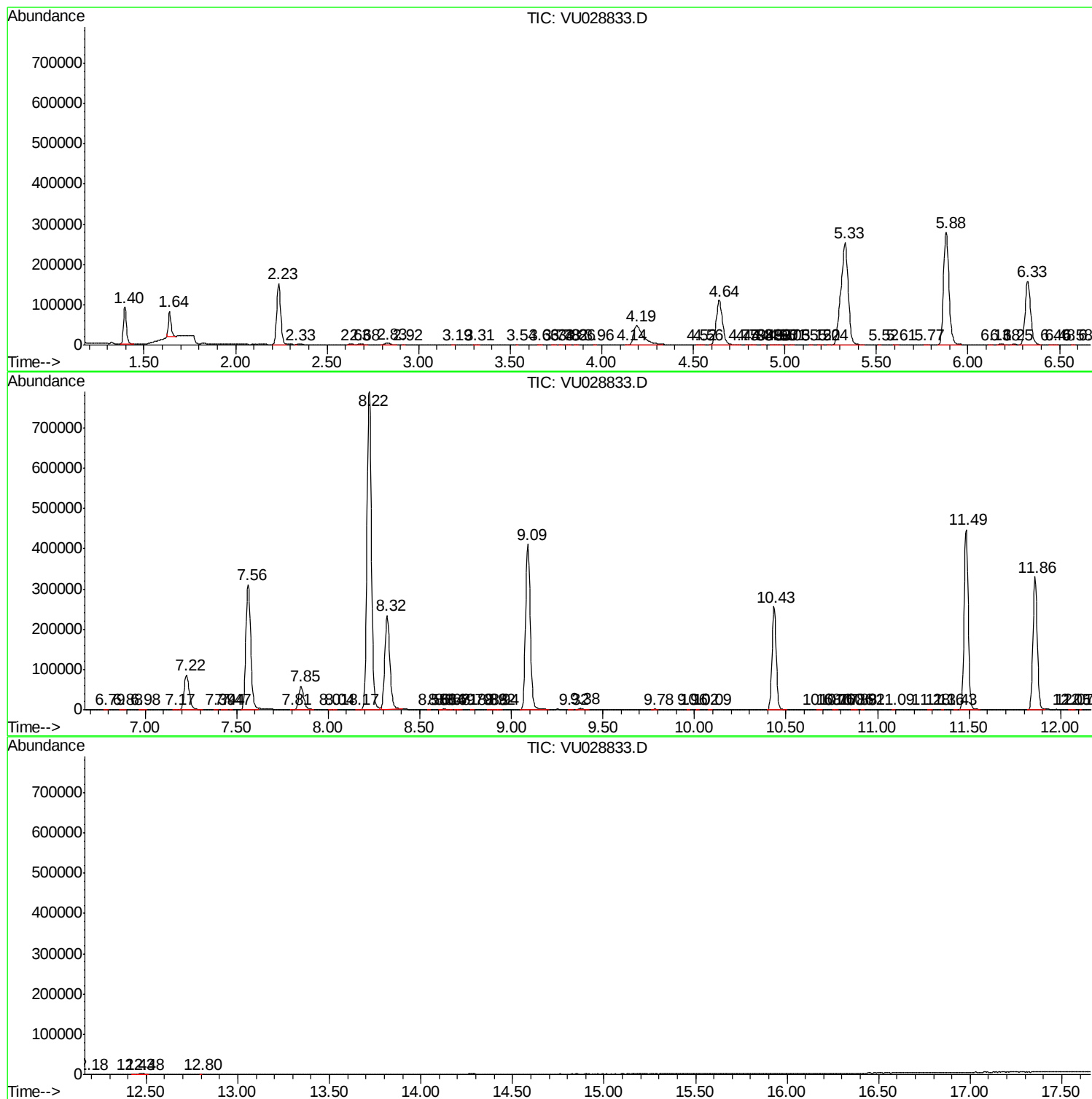
Sum of corrected areas: 7523666

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU122018\
Data File : VU028833.D
Acq On : 20 Dec 2018 18:42
Operator : MD/SY
Sample : J6419-14ME
Misc : 5.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BF042ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU122018\
Data File : VU028833.D
Acq On : 20 Dec 2018 18:42
Operator : MD/SY
Sample : J6419-14ME
Misc : 5.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BF042ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU122018\
Data File : VU028833.D
Acq On : 20 Dec 2018 18:42
Operator : MD/SY
Sample : J6419-14ME
Misc : 5.28g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BF042ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM122018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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