

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU012920\
 Data File : VU036585.D
 Acq On : 29 Jan 2020 11:44
 Operator : JC/MD
 Sample : VU0129MBL01
 Misc : 5.00µL/5.0mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK48

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\SOMULM012920WMA.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	1.616	79	86	98	rVB	149108	154637	15.17%	2.004%
2	1.932	177	184	199	rVB	121469	151662	14.87%	1.965%
3	2.594	377	390	405	rBV	215347	353951	34.71%	4.587%
4	2.822	455	461	474	rVB2	637	999	0.10%	0.013%
5	2.925	490	493	494	rBV	154	91	0.01%	0.001%
6	2.983	507	511	514	rBV	228	149	0.01%	0.002%
7	3.083	533	542	549	rBV3	1431	2283	0.22%	0.030%
8	3.128	554	556	558	rBV	137	61	0.01%	0.001%
9	3.160	564	566	571	rVB	225	113	0.01%	0.001%
10	3.227	578	587	598	rVB3	804	1693	0.17%	0.022%
11	3.269	598	600	607	rVB	207	112	0.01%	0.001%
12	3.314	607	614	618	rBV	151	179	0.02%	0.002%
13	3.401	638	641	645	rBV	78	53	0.01%	0.001%
14	3.420	645	647	649	rBV	141	45	0.00%	0.001%
15	3.459	656	659	661	rBV	70	50	0.00%	0.001%
16	3.501	669	672	676	rBV	91	80	0.01%	0.001%
17	3.645	714	717	720	rBV	177	137	0.01%	0.002%
18	3.864	782	785	787	rBV	81	55	0.01%	0.001%
19	3.941	805	809	811	rBV	90	66	0.01%	0.001%
20	3.973	817	819	822	rBV	75	38	0.00%	0.000%
21	3.996	823	826	829	rBV2	201	126	0.01%	0.002%
22	4.057	841	845	846	rBV	95	68	0.01%	0.001%
23	4.137	866	870	872	rBV	106	74	0.01%	0.001%
24	4.243	900	903	908	rVB	154	123	0.01%	0.002%
25	4.279	908	914	917	rBV	99	136	0.01%	0.002%
26	4.321	924	927	930	rBV	146	74	0.01%	0.001%
27	4.394	947	950	954	rBV2	149	147	0.01%	0.002%
28	4.468	969	973	976	rVV	103	80	0.01%	0.001%
29	4.555	998	1000	1004	rBV2	130	91	0.01%	0.001%
30	4.578	1004	1007	1010	rVV2	132	84	0.01%	0.001%
31	4.677	1022	1038	1083	rBV	91663	224929	22.06%	2.915%
32	5.111	1156	1173	1193	rBV	172338	378600	37.13%	4.906%
33	5.266	1218	1221	1223	rBV	216	178	0.02%	0.002%
34	5.324	1235	1239	1240	rBV	495	357	0.04%	0.005%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU012920\
 Data File : VU036585.D
 Acq On : 29 Jan 2020 11:44
 Operator : JC/MD
 Sample : VU0129MBL01
 Misc : 5.00µ/5.0mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK48

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\SOMULM012920WMA.M
 Title : VOC Analysis

35	5.382	1253	1257	1260	rBV	81	78	0.01%	0.001%
36	5.410	1260	1266	1267	rBV2	420	403	0.04%	0.005%
37	5.484	1286	1289	1292	rBV	63	47	0.00%	0.001%
38	5.504	1293	1295	1297	rVV	181	91	0.01%	0.001%
39	5.591	1319	1322	1324	rBV	83	46	0.00%	0.001%
40	5.681	1347	1350	1353	rBV	77	48	0.00%	0.001%
41	5.767	1356	1377	1404	rBV2	392102	1019694	100.00%	13.214%
42	6.070	1469	1471	1473	rBV2	167	99	0.01%	0.001%
43	6.189	1503	1508	1511	rBV2	205	258	0.03%	0.003%
44	6.288	1523	1539	1557	rBV	335175	629504	61.73%	8.157%
45	6.565	1616	1625	1634	rVB5	2351	4311	0.42%	0.056%
46	6.729	1661	1676	1698	rBV	235510	450140	44.14%	5.833%
47	6.880	1721	1723	1728	rVV	133	94	0.01%	0.001%
48	6.909	1728	1732	1734	rVB	107	69	0.01%	0.001%
49	6.938	1740	1741	1744	rVB	255	82	0.01%	0.001%
50	6.954	1744	1746	1748	rVB	134	51	0.01%	0.001%
51	6.970	1748	1751	1753	rBV	169	98	0.01%	0.001%
52	7.021	1765	1767	1771	rVB	155	70	0.01%	0.001%
53	7.176	1811	1815	1818	rVB	56	46	0.00%	0.001%
54	7.214	1818	1827	1840	rBV4	1444	2351	0.23%	0.030%
55	7.263	1840	1842	1846	rVB	69	44	0.00%	0.001%
56	7.285	1846	1849	1853	rBV	158	91	0.01%	0.001%
57	7.304	1853	1855	1857	rBV	74	42	0.00%	0.001%
58	7.343	1863	1867	1870	rBV	57	47	0.00%	0.001%
59	7.365	1870	1874	1878	rVV	72	70	0.01%	0.001%
60	7.423	1889	1892	1894	rBV	85	55	0.01%	0.001%
61	7.481	1906	1910	1913	rBV	91	80	0.01%	0.001%
62	7.600	1932	1947	1966	rBV	133297	233358	22.89%	3.024%
63	7.931	2035	2050	2080	rBV	503982	885972	86.89%	11.481%
64	8.140	2112	2115	2117	rBV	64	43	0.00%	0.001%
65	8.211	2124	2137	2157	rBV	88503	153749	15.08%	1.992%
66	8.391	2190	2193	2195	rBV	70	43	0.00%	0.001%
67	8.510	2227	2230	2232	rBV	83	56	0.01%	0.001%
68	8.565	2246	2247	2249	rVB	146	54	0.01%	0.001%
69	8.584	2250	2253	2257	rVB	200	113	0.01%	0.001%
70	8.671	2266	2280	2324	rBV	223356	509861	50.00%	6.607%
71	8.825	2326	2328	2331	rVB2	213	124	0.01%	0.002%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU012920\
 Data File : VU036585.D
 Acq On : 29 Jan 2020 11:44
 Operator : JC/MD
 Sample : VU0129MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK48

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\SOMULM012920WMA.M
 Title : VOC Analysis

72	8.844	2331	2334	2337	rBV	96	74	0.01%	0.001%
73	8.925	2357	2359	2360	rBV	123	53	0.01%	0.001%
74	8.941	2362	2364	2369	rVB	166	69	0.01%	0.001%
75	9.021	2386	2389	2391	rBV	126	84	0.01%	0.001%
76	9.124	2420	2421	2422	rBV	165	35	0.00%	0.000%
77	9.253	2457	2461	2464	rBV	233	109	0.01%	0.001%
78	9.327	2482	2484	2487	rBV2	119	85	0.01%	0.001%
79	9.446	2508	2521	2557	rVB	439333	751639	73.71%	9.740%
80	9.571	2558	2560	2562	rBV	78	39	0.00%	0.001%
81	9.594	2562	2567	2579	rBV3	591	853	0.08%	0.011%
82	9.680	2590	2594	2598	rBV	89	100	0.01%	0.001%
83	9.716	2599	2605	2613	rVV3	489	771	0.08%	0.010%
84	9.799	2625	2631	2633	rBV2	207	135	0.01%	0.002%
85	9.934	2671	2673	2674	rBV2	129	53	0.01%	0.001%
86	10.031	2699	2703	2705	rBV	110	93	0.01%	0.001%
87	10.089	2720	2721	2723	rBV	102	46	0.00%	0.001%
88	10.108	2726	2727	2728	rVV	225	76	0.01%	0.001%
89	10.131	2732	2734	2743	rVB4	678	627	0.06%	0.008%
90	10.394	2813	2816	2820	rBV	139	102	0.01%	0.001%
91	10.504	2847	2850	2851	rBV2	278	179	0.02%	0.002%
92	10.629	2887	2889	2890	rBV2	142	58	0.01%	0.001%
93	10.658	2895	2898	2902	rVB	205	132	0.01%	0.002%
94	10.783	2923	2937	2955	rBV	315892	524919	51.48%	6.802%
95	10.999	3002	3004	3007	rBV	227	140	0.01%	0.002%
96	11.089	3030	3032	3035	rVB	170	77	0.01%	0.001%
97	11.835	3251	3264	3282	rVB	358287	601992	59.04%	7.801%
98	12.217	3369	3383	3402	rBV	400485	671065	65.81%	8.696%
99	12.294	3405	3407	3413	rVB	186	166	0.02%	0.002%
100	13.709	3844	3847	3852	rBV2	264	232	0.02%	0.003%

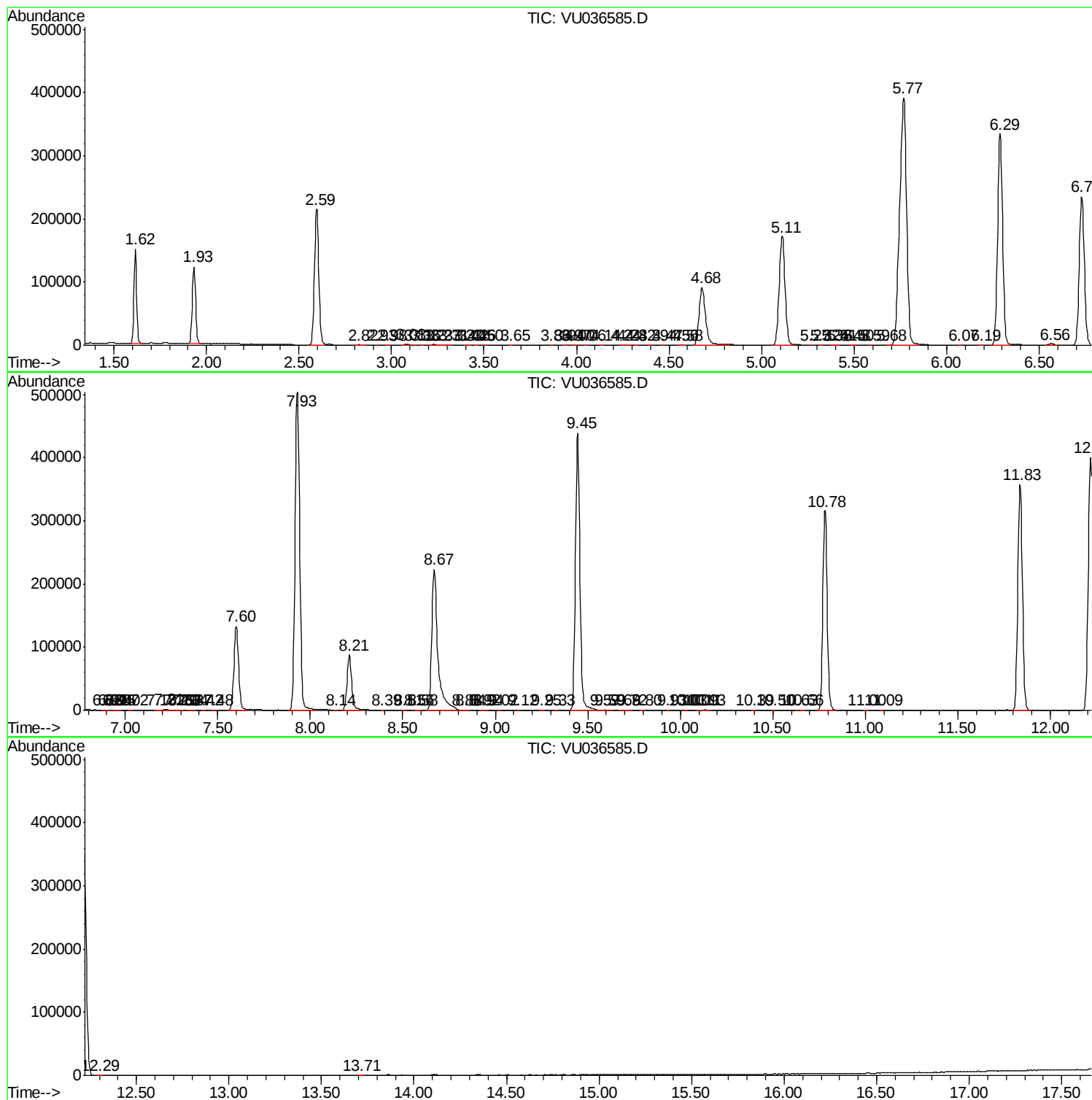
Sum of corrected areas: 7716906

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU012920\
Data File : VU036585.D
Acq On : 29 Jan 2020 11:44
Operator : JC/MD
Sample : VU0129MBL01
Misc : 5.00q/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK48

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM012920WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSV0A_U\DATA\VU012920\
Data File : VU036585.D
Acq On : 29 Jan 2020 11:44
Operator : JC/MD
Sample : VU0129MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSV0A_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSV0A_U
ClientSampleId :
VBLK48

Quant Method : Z:\V0ASRV\HPCHEM1\MSV0A_U\METHOD\SOMULM012920WMA.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\VU012920\
Data File : VU036585.D
Acq On : 29 Jan 2020 11:44
Operator : JC/MD
Sample : VU0129MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK48

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM012920WMA.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