

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101921\
 Data File : VU045332.D
 Acq On : 19 Oct 2021 16:12
 Operator : SY/MD
 Sample : VU1019MBL02
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK026

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\SFAMULM101921WMA.M
 Title : VOC Analysis

Signal : TIC: VU045332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.462	32	38	53	rBV	16200	30157	3.29%	0.362%
2	1.601	74	81	96	rBV	80147	88830	9.70%	1.066%
3	1.874	160	166	173	rBV	36516	40032	4.37%	0.480%
4	2.494	357	359	363	rVB	303	166	0.02%	0.002%
5	2.549	364	376	399	rBV2	114999	201598	22.02%	2.419%
6	2.671	411	414	420	rBV2	161	214	0.02%	0.003%
7	2.726	424	431	433	rBV2	163	175	0.02%	0.002%
8	2.781	438	448	457	rVB2	1170	1891	0.21%	0.023%
9	2.864	470	474	476	rBV2	220	157	0.02%	0.002%
10	2.887	476	481	487	rVB	283	373	0.04%	0.004%
11	2.919	487	491	494	rBV	234	221	0.02%	0.003%
12	2.957	494	503	513	rBV3	2468	4328	0.47%	0.052%
13	3.044	523	530	535	rBV2	1010	1484	0.16%	0.018%
14	3.189	570	575	579	rVB2	291	275	0.03%	0.003%
15	3.347	622	624	629	rVB	459	375	0.04%	0.005%
16	3.549	684	687	690	rVB2	185	125	0.01%	0.002%
17	3.629	707	712	716	rBV	150	193	0.02%	0.002%
18	4.064	843	847	848	rBV2	213	135	0.01%	0.002%
19	4.285	913	916	920	rBV2	152	151	0.02%	0.002%
20	4.559	997	1001	1004	rBV2	224	147	0.02%	0.002%
21	4.633	1009	1024	1054	rBV	130160	330865	36.13%	3.971%
22	4.816	1078	1081	1089	rVB3	208	287	0.03%	0.003%
23	4.871	1094	1098	1100	rBV2	188	189	0.02%	0.002%
24	4.977	1126	1131	1134	rBV2	124	131	0.01%	0.002%
25	5.067	1142	1159	1178	rBV	173676	379078	41.40%	4.549%
26	5.295	1222	1230	1235	rVB2	552	905	0.10%	0.011%
27	5.372	1249	1254	1261	rVB3	452	633	0.07%	0.008%
28	5.652	1336	1341	1342	rBV2	194	178	0.02%	0.002%
29	5.723	1342	1363	1389	rVV2	315832	867047	94.69%	10.405%
30	5.919	1421	1424	1428	rVB2	255	207	0.02%	0.002%
31	5.944	1428	1432	1434	rBV	194	170	0.02%	0.002%
32	5.973	1434	1441	1442	rBV4	1615	1519	0.17%	0.018%
33	6.118	1481	1486	1491	rBV2	400	428	0.05%	0.005%
34	6.250	1512	1527	1548	rBV	368031	689065	75.25%	8.269%
35	6.427	1577	1582	1585	rBV3	172	179	0.02%	0.002%
36	6.526	1606	1613	1625	rVB4	2865	5321	0.58%	0.064%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101921\
 Data File : VU045332.D
 Acq On : 19 Oct 2021 16:12
 Operator : SY/MD
 Sample : VU1019MBL02
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK026

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\SFAMULM101921WMA.M
 Title : VOC Analysis

37	6.597	1625	1635	1645	rBV3	1665	3129	0.34%	0.038%
38	6.694	1650	1665	1684	rBV	228333	445619	48.67%	5.348%
39	6.806	1695	1700	1707	rVB3	431	607	0.07%	0.007%
40	6.951	1741	1745	1750	rVB2	139	122	0.01%	0.001%
41	7.051	1768	1776	1777	rBV2	539	584	0.06%	0.007%
42	7.115	1793	1796	1799	rVV	197	156	0.02%	0.002%
43	7.176	1807	1815	1828	rVB4	1903	3312	0.36%	0.040%
44	7.224	1828	1830	1837	rVB2	171	143	0.02%	0.002%
45	7.269	1841	1844	1845	rBV	178	122	0.01%	0.001%
46	7.378	1874	1878	1881	rVB2	146	121	0.01%	0.001%
47	7.417	1887	1890	1892	rBV	167	122	0.01%	0.001%
48	7.469	1903	1906	1910	rBV	161	141	0.02%	0.002%
49	7.568	1925	1937	1954	rBV	130458	227036	24.79%	2.725%
50	7.694	1969	1976	1983	rBB5	724	982	0.11%	0.012%
51	7.800	2000	2009	2017	rBV3	1864	2974	0.32%	0.036%
52	7.899	2026	2040	2055	rBV	343601	587849	64.20%	7.054%
53	7.973	2056	2063	2078	rVB3	5029	10793	1.18%	0.130%
54	8.076	2094	2095	2099	rVB	309	166	0.02%	0.002%
55	8.105	2099	2104	2106	rBV	274	273	0.03%	0.003%
56	8.182	2116	2128	2146	rBV	98285	167244	18.26%	2.007%
57	8.485	2218	2222	2224	rBV2	198	142	0.02%	0.002%
58	8.552	2241	2243	2246	rBV2	168	121	0.01%	0.001%
59	8.642	2258	2271	2308	rBV	459826	848724	92.69%	10.185%
60	9.208	2444	2447	2452	rBV2	133	126	0.01%	0.002%
61	9.420	2500	2513	2533	rBV	563702	915684	100.00%	10.989%
62	9.578	2553	2562	2567	rBV4	727	1073	0.12%	0.013%
63	9.648	2577	2584	2587	rBV2	320	417	0.05%	0.005%
64	9.697	2591	2599	2606	rVB3	1237	1849	0.20%	0.022%
65	9.935	2668	2673	2676	rBV2	240	298	0.03%	0.004%
66	10.041	2701	2706	2710	rBV2	251	262	0.03%	0.003%
67	10.115	2719	2729	2737	rBV3	1032	1661	0.18%	0.020%
68	10.253	2766	2772	2774	rBV2	191	254	0.03%	0.003%
69	10.298	2778	2786	2789	rBV	265	347	0.04%	0.004%
70	10.484	2840	2844	2853	rVB	434	591	0.06%	0.007%
71	10.636	2888	2891	2898	rVB	609	591	0.06%	0.007%
72	10.677	2902	2904	2907	rVB	332	192	0.02%	0.002%
73	10.703	2907	2912	2915	rBV2	218	224	0.02%	0.003%
74	10.761	2917	2930	2946	rBV	475852	760871	83.09%	9.131%
75	11.095	3027	3034	3041	rVB2	693	943	0.10%	0.011%
76	11.353	3105	3114	3116	rBV2	197	274	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101921\
 Data File : VU045332.D
 Acq On : 19 Oct 2021 16:12
 Operator : SY/MD
 Sample : VU1019MBL02
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK026

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\SFAMULM101921WMA.M
 Title : VOC Analysis

77	11.414	3129	3133	3136	rBV2	242	205	0.02%	0.002%
78	11.475	3146	3152	3158	rBV2	1507	1940	0.21%	0.023%
79	11.751	3232	3238	3244	rBV3	1715	2016	0.22%	0.024%
80	11.816	3245	3258	3276	rBV	530984	833442	91.02%	10.002%
81	11.951	3298	3300	3303	rVB2	255	123	0.01%	0.001%
82	11.973	3305	3307	3314	rVB2	323	297	0.03%	0.004%
83	12.198	3357	3377	3393	rBV	513525	820242	89.58%	9.843%
84	12.349	3421	3424	3426	rBV	186	130	0.01%	0.002%
85	12.446	3450	3454	3457	rBV2	269	262	0.03%	0.003%
86	12.542	3481	3484	3489	rBV2	196	243	0.03%	0.003%
87	12.626	3507	3510	3512	rBV	169	125	0.01%	0.002%
88	12.799	3562	3564	3567	rBV2	193	147	0.02%	0.002%
89	12.999	3622	3626	3634	rVB4	482	578	0.06%	0.007%
90	13.082	3648	3652	3654	rBV	183	165	0.02%	0.002%
91	13.224	3690	3696	3706	rBV3	2331	3174	0.35%	0.038%
92	13.311	3718	3723	3727	rBV2	222	247	0.03%	0.003%
93	13.391	3744	3748	3750	rBV2	307	229	0.03%	0.003%
94	13.455	3765	3768	3770	rBV	202	171	0.02%	0.002%
95	13.607	3809	3815	3817	rBV2	281	324	0.04%	0.004%
96	13.655	3827	3830	3834	rBV	239	179	0.02%	0.002%
97	13.844	3882	3889	3900	rVB2	4836	7565	0.83%	0.091%
98	14.092	3955	3966	3978	rBV	11292	18704	2.04%	0.224%
99	14.333	4034	4041	4052	rVB4	6009	8658	0.95%	0.104%
100	15.346	4350	4356	4360	rBV3	411	519	0.06%	0.006%

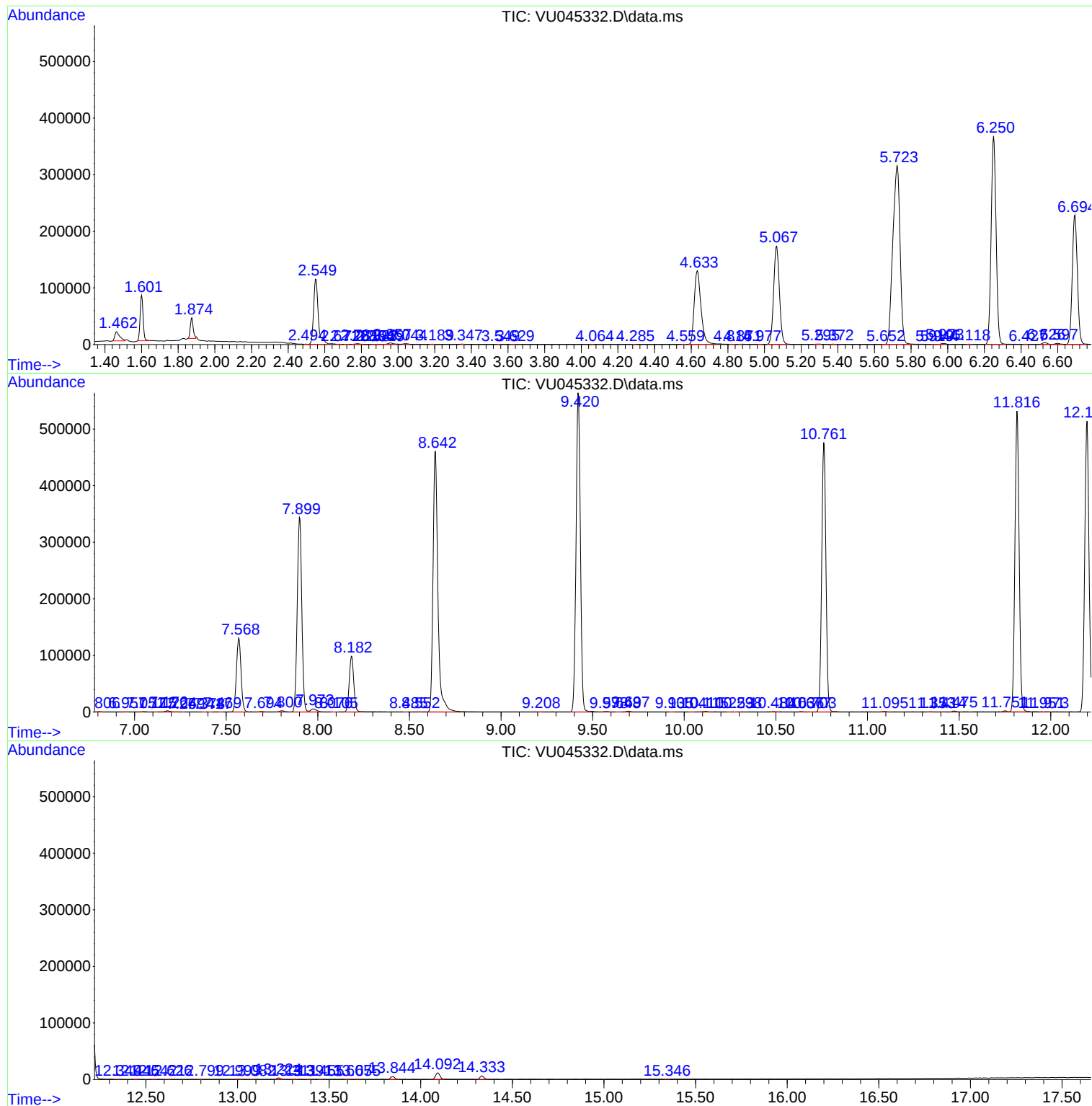
Sum of corrected areas: 8333053

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101921\
Data File : VU045332.D
Acq On : 19 Oct 2021 16:12
Operator : SY/MD
Sample : VU1019MBL02
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK026

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101921WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101921\
Data File : VU045332.D
Acq On : 19 Oct 2021 16:12
Operator : SY/MD
Sample : VU1019MBL02
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK026

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101921WMA.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\VU101921\
Data File : VU045332.D
Acq On : 19 Oct 2021 16:12
Operator : SY/MD
Sample : VU1019MBL02
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK026

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101921WMA.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
