

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046443.D
 Acq On : 17 Dec 2021 00:25
 Operator : SY/MD
 Sample : M5101-07MEDL 40X
 Misc : 6.38g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL28MEDL

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: VU046443.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	102	rBV	59551	75179	14.75%	1.750%
2	1.919	171	180	194	rBV	41131	58181	11.41%	1.354%
3	2.080	225	230	233	rBV2	274	318	0.06%	0.007%
4	2.176	257	260	263	rVB	184	130	0.03%	0.003%
5	2.192	263	265	268	rBV2	179	109	0.02%	0.003%
6	2.250	281	283	287	rVB2	208	151	0.03%	0.004%
7	2.501	357	361	363	rBV	152	150	0.03%	0.003%
8	2.572	371	383	412	rBV	107234	179497	35.21%	4.177%
9	2.710	423	426	429	rBB	174	144	0.03%	0.003%
10	2.787	447	450	452	rBV2	270	210	0.04%	0.005%
11	2.803	452	455	458	rVV2	256	201	0.04%	0.005%
12	2.832	461	464	467	rBV	157	154	0.03%	0.004%
13	2.919	489	491	494	rBB	143	96	0.02%	0.002%
14	2.957	499	503	505	rBB	154	127	0.02%	0.003%
15	2.980	506	510	512	rBB	152	100	0.02%	0.002%
16	3.057	525	534	538	rBV2	965	1354	0.27%	0.032%
17	3.192	563	576	593	rBB2	5584	12702	2.49%	0.296%
18	3.308	609	612	614	rBV	138	121	0.02%	0.003%
19	3.681	725	728	730	rBB	156	100	0.02%	0.002%
20	3.909	797	799	802	rBV	126	113	0.02%	0.003%
21	3.983	819	822	824	rBB	148	101	0.02%	0.002%
22	4.636	1011	1025	1057	rBV	45677	123715	24.27%	2.879%
23	4.842	1084	1089	1094	rVB2	288	376	0.07%	0.009%
24	4.890	1102	1104	1107	rBB	153	106	0.02%	0.002%
25	4.986	1131	1134	1136	rBB	156	105	0.02%	0.002%
26	5.067	1144	1159	1180	rBV	93918	203971	40.02%	4.747%
27	5.266	1218	1221	1225	rVB	172	110	0.02%	0.003%
28	5.292	1225	1229	1230	rBV2	392	208	0.04%	0.005%
29	5.314	1234	1236	1239	rVB2	282	179	0.04%	0.004%
30	5.346	1239	1246	1249	rBV2	322	418	0.08%	0.010%
31	5.591	1318	1322	1325	rBB	187	175	0.03%	0.004%
32	5.729	1342	1365	1387	rBV2	189944	509727	100.00%	11.863%
33	6.253	1514	1528	1559	rVB	179938	334920	65.71%	7.794%
34	6.363	1560	1562	1565	rBB	209	103	0.02%	0.002%
35	6.417	1576	1579	1581	rBV	143	122	0.02%	0.003%
36	6.543	1609	1618	1630	rBB5	14192	26403	5.18%	0.614%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046443.D
 Acq On : 17 Dec 2021 00:25
 Operator : SY/MD
 Sample : M5101-07MEDL 40X
 Misc : 6.38g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL28MEDL

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	6.588	1630	1632	1635	rBV	146	117	0.02%	0.003%
38	6.694	1652	1665	1684	rBV	118541	227635	44.66%	5.298%
39	6.880	1720	1723	1728	rBV	166	204	0.04%	0.005%
40	7.192	1817	1820	1823	rVB2	318	256	0.05%	0.006%
41	7.366	1872	1874	1878	rVB	152	128	0.03%	0.003%
42	7.427	1890	1893	1895	rBV	145	120	0.02%	0.003%
43	7.449	1898	1900	1903	rBB	150	102	0.02%	0.002%
44	7.568	1925	1937	1959	rBB	61477	105691	20.73%	2.460%
45	7.690	1973	1975	1977	rBV	325	147	0.03%	0.003%
46	7.764	1995	1998	2000	rBV	134	114	0.02%	0.003%
47	7.787	2000	2005	2011	rVB2	538	637	0.12%	0.015%
48	7.845	2021	2023	2027	rBV	149	152	0.03%	0.004%
49	7.899	2027	2040	2055	rVV	231426	394081	77.31%	9.171%
50	7.970	2057	2062	2075	rVB2	3378	5581	1.09%	0.130%
51	8.102	2101	2103	2106	rBB	142	98	0.02%	0.002%
52	8.179	2117	2127	2145	rVB	42835	70590	13.85%	1.643%
53	8.269	2150	2155	2157	rBV	242	250	0.05%	0.006%
54	8.292	2160	2162	2164	rBV	240	135	0.03%	0.003%
55	8.478	2212	2220	2221	rBV2	565	571	0.11%	0.013%
56	8.555	2232	2244	2257	rVB	105733	176573	34.64%	4.109%
57	8.636	2257	2269	2285	rBV	149937	253330	49.70%	5.896%
58	8.764	2307	2309	2313	rVB2	152	130	0.03%	0.003%
59	8.825	2323	2328	2331	rBV	151	196	0.04%	0.005%
60	8.874	2340	2343	2346	rBV	180	159	0.03%	0.004%
61	8.915	2349	2356	2363	rVV2	727	912	0.18%	0.021%
62	8.948	2363	2366	2369	rVB	173	145	0.03%	0.003%
63	9.105	2412	2415	2417	rBV	115	103	0.02%	0.002%
64	9.144	2424	2427	2432	rBV	179	209	0.04%	0.005%
65	9.417	2500	2512	2538	rVV	267085	433290	85.00%	10.084%
66	9.542	2548	2551	2554	rBV	149	141	0.03%	0.003%
67	9.568	2555	2559	2566	rVB2	353	503	0.10%	0.012%
68	9.697	2592	2599	2605	rBV3	724	1082	0.21%	0.025%
69	9.948	2674	2677	2682	rBV	160	203	0.04%	0.005%
70	10.102	2721	2725	2729	rVB2	449	397	0.08%	0.009%
71	10.472	2836	2840	2845	rBV	218	293	0.06%	0.007%
72	10.665	2896	2900	2901	rBV	500	255	0.05%	0.006%
73	10.758	2917	2929	2946	rVB	167585	267884	52.55%	6.234%
74	11.150	3047	3051	3054	rBV	162	181	0.04%	0.004%
75	11.452	3140	3145	3147	rBV2	299	220	0.04%	0.005%
76	11.468	3147	3150	3151	rBV	226	150	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046443.D
 Acq On : 17 Dec 2021 00:25
 Operator : SY/MD
 Sample : M5101-07MEDL 40X
 Misc : 6.38g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL28MEDL

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	11.555	3172	3177	3180	rBB	202	195	0.04%	0.005%
78	11.697	3217	3221	3225	rVB2	177	141	0.03%	0.003%
79	11.812	3245	3257	3273	rBV	287106	442705	86.85%	10.303%
80	11.944	3295	3298	3303	rVV2	376	343	0.07%	0.008%
81	11.973	3304	3307	3313	rVB2	420	421	0.08%	0.010%
82	12.005	3313	3317	3320	rBV	151	113	0.02%	0.003%
83	12.063	3331	3335	3338	rBV	182	209	0.04%	0.005%
84	12.195	3364	3376	3390	rVV	236963	375162	73.60%	8.731%
85	12.481	3460	3465	3473	rBV	217	410	0.08%	0.010%
86	12.562	3486	3490	3495	rBV	94	101	0.02%	0.002%
87	12.774	3549	3556	3565	rBV3	575	902	0.18%	0.021%
88	13.372	3739	3742	3746	rBV	146	117	0.02%	0.003%
89	13.864	3890	3895	3898	rBV	128	110	0.02%	0.003%
90	13.886	3899	3902	3905	rBV	106	98	0.02%	0.002%
91	14.095	3964	3967	3970	rVB	230	182	0.04%	0.004%
92	14.285	4023	4026	4029	rBV	138	116	0.02%	0.003%
93	14.581	4109	4118	4126	rVB2	809	1315	0.26%	0.031%
94	15.497	4400	4403	4407	rVB	257	173	0.03%	0.004%
95	15.523	4407	4411	4415	rBV2	214	156	0.03%	0.004%
96	15.642	4446	4448	4452	rBV2	150	133	0.03%	0.003%
97	15.674	4454	4458	4463	rBV	221	223	0.04%	0.005%
98	15.841	4505	4510	4513	rBV2	234	216	0.04%	0.005%
99	15.951	4540	4544	4547	rBV2	214	245	0.05%	0.006%
100	17.304	4963	4965	4969	rBV	388	272	0.05%	0.006%

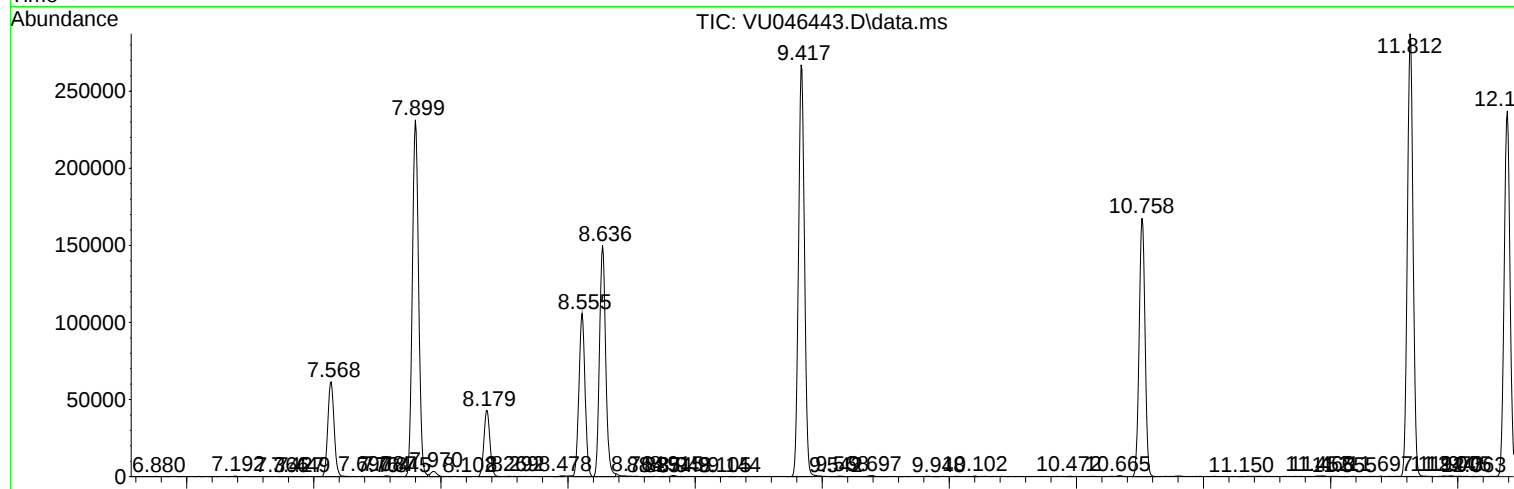
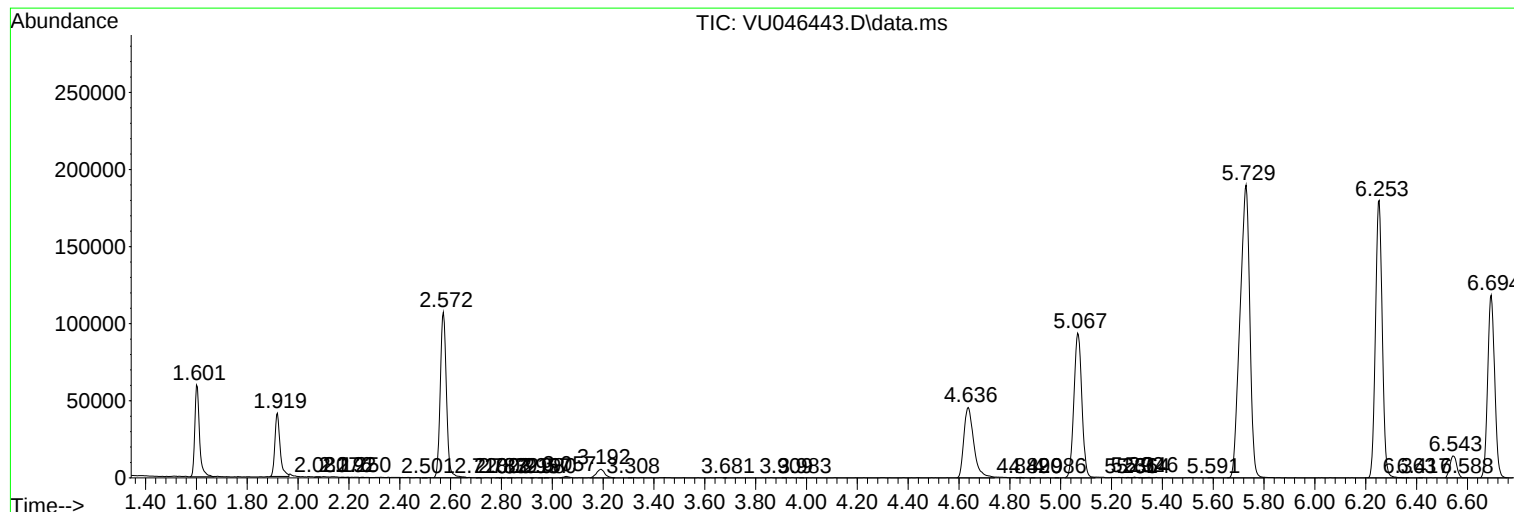
Sum of corrected areas: 4296899

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
Data File : VU046443.D
Acq On : 17 Dec 2021 00:25
Operator : SY/MD
Sample : M5101-07MEDL 40X
Misc : 6.38g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL28MEDL

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
Data File : VU046443.D
Acq On : 17 Dec 2021 00:25
Operator : SY/MD
Sample : M5101-07MEDL 40X
Misc : 6.38g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL28MEDL

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\VU121621\
Data File : VU046443.D
Acq On : 17 Dec 2021 00:25
Operator : SY/MD
Sample : M5101-07MEDL 40X
Misc : 6.38g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL28MEDL

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	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------