

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046444.D
 Acq On : 17 Dec 2021 00:47
 Operator : SY/MD
 Sample : M5101-13ME 20X
 Misc : 6.93g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL37ME

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: VU046444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	73	82	109	rVB	59854	75826	14.98%	1.840%
2	1.919	171	180	203	rBV	40826	60617	11.97%	1.471%
3	2.330	305	308	313	rVB	258	196	0.04%	0.005%
4	2.359	314	317	320	rBV	151	115	0.02%	0.003%
5	2.572	371	383	405	rBV	108501	178441	35.24%	4.331%
6	2.800	451	454	459	rBV2	297	314	0.06%	0.008%
7	2.893	480	483	487	rBV	138	171	0.03%	0.004%
8	2.961	500	504	507	rBB	142	118	0.02%	0.003%
9	3.054	527	533	538	rBB2	655	826	0.16%	0.020%
10	3.086	539	543	546	rBB	165	150	0.03%	0.004%
11	3.192	564	576	589	rBB	3402	7283	1.44%	0.177%
12	3.301	606	610	614	rBB	143	120	0.02%	0.003%
13	3.327	615	618	622	rBV	143	173	0.03%	0.004%
14	3.700	731	734	736	rBV	128	112	0.02%	0.003%
15	3.848	778	780	784	rBB	142	126	0.02%	0.003%
16	4.366	938	941	944	rBB	144	123	0.02%	0.003%
17	4.449	965	967	970	rVB	174	115	0.02%	0.003%
18	4.549	996	998	1002	rBB	123	111	0.02%	0.003%
19	4.636	1011	1025	1059	rBV	45487	119895	23.68%	2.910%
20	4.797	1072	1075	1078	rVB2	177	121	0.02%	0.003%
21	4.893	1102	1105	1107	rBB2	269	167	0.03%	0.004%
22	5.067	1143	1159	1179	rBV	92879	203233	40.14%	4.933%
23	5.202	1199	1201	1206	rVB	300	237	0.05%	0.006%
24	5.237	1207	1212	1215	rBV	346	378	0.07%	0.009%
25	5.263	1215	1220	1222	rVV2	259	249	0.05%	0.006%
26	5.321	1226	1238	1250	rVV3	5893	12215	2.41%	0.296%
27	5.729	1344	1365	1385	rBV2	187984	506293	100.00%	12.289%
28	6.253	1513	1528	1555	rBV	175345	332119	65.60%	8.061%
29	6.350	1555	1558	1560	rVV2	312	244	0.05%	0.006%
30	6.494	1599	1603	1607	rBB	168	187	0.04%	0.005%
31	6.542	1611	1618	1627	rBB8	2253	3857	0.76%	0.094%
32	6.694	1651	1665	1685	rBV	116402	226911	44.82%	5.507%
33	7.179	1813	1816	1817	rBV	168	116	0.02%	0.003%
34	7.568	1926	1937	1958	rVV	61389	104441	20.63%	2.535%
35	7.655	1961	1964	1967	rBB	133	116	0.02%	0.003%
36	7.806	2007	2011	2014	rBV	125	137	0.03%	0.003%

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 Title : VOC Analysis

37	7.899	2027	2040	2055	rVV	229553	389497	76.93%	9.454%
38	7.970	2057	2062	2075	rVB2	2983	4816	0.95%	0.117%
39	8.057	2086	2089	2092	rBB	151	127	0.03%	0.003%
40	8.179	2116	2127	2142	rBV	42928	70477	13.92%	1.711%
41	8.256	2146	2151	2153	rBV2	264	275	0.05%	0.007%
42	8.285	2157	2160	2163	rBV2	264	283	0.06%	0.007%
43	8.388	2190	2192	2195	rBV	151	136	0.03%	0.003%
44	8.475	2212	2219	2222	rVV	423	465	0.09%	0.011%
45	8.555	2232	2244	2257	rVB2	31974	54242	10.71%	1.317%
46	8.636	2257	2269	2295	rVV	146579	248059	49.00%	6.021%
47	8.732	2295	2299	2303	rVV3	329	298	0.06%	0.007%
48	8.890	2344	2348	2351	rBV	140	144	0.03%	0.003%
49	8.915	2351	2356	2362	rBV2	389	401	0.08%	0.010%
50	8.964	2368	2371	2374	rBV	143	145	0.03%	0.004%
51	9.021	2386	2389	2392	rBB	133	112	0.02%	0.003%
52	9.044	2393	2396	2398	rBV	179	143	0.03%	0.003%
53	9.076	2402	2406	2409	rBB	135	138	0.03%	0.003%
54	9.176	2433	2437	2440	rBV	169	199	0.04%	0.005%
55	9.279	2462	2469	2471	rBV	168	214	0.04%	0.005%
56	9.308	2475	2478	2481	rBV	142	150	0.03%	0.004%
57	9.362	2492	2495	2497	rBV	160	137	0.03%	0.003%
58	9.420	2500	2513	2535	rVV	264691	430028	84.94%	10.437%
59	9.574	2557	2561	2564	rVB2	280	222	0.04%	0.005%
60	9.703	2596	2601	2606	rVB2	349	436	0.09%	0.011%
61	9.803	2627	2632	2637	rBB	132	183	0.04%	0.004%
62	9.828	2637	2640	2643	rBV	157	153	0.03%	0.004%
63	9.893	2658	2660	2664	rBV	161	160	0.03%	0.004%
64	9.915	2664	2667	2670	rVB	183	154	0.03%	0.004%
65	9.941	2671	2675	2683	rBB	164	303	0.06%	0.007%
66	9.976	2683	2686	2689	rBV	140	137	0.03%	0.003%
67	10.150	2733	2740	2742	rBV	157	227	0.04%	0.006%
68	10.234	2763	2766	2769	rBV	154	157	0.03%	0.004%
69	10.301	2784	2787	2789	rBV	158	137	0.03%	0.003%
70	10.407	2817	2820	2824	rBV	161	187	0.04%	0.005%
71	10.465	2834	2838	2841	rBB	155	156	0.03%	0.004%
72	10.504	2846	2850	2852	rBV	168	165	0.03%	0.004%
73	10.568	2867	2870	2875	rBB	174	194	0.04%	0.005%
74	10.629	2886	2889	2895	rVB	181	223	0.04%	0.005%
75	10.671	2896	2902	2908	rBV	793	776	0.15%	0.019%
76	10.758	2917	2929	2943	rVB	168546	267499	52.83%	6.493%

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77	10.877	2964	2966	2968	rVB	238	119	0.02%	0.003%
78	10.899	2968	2973	2981	rBV2	405	747	0.15%	0.018%
79	11.095	3027	3034	3038	rBV	158	282	0.06%	0.007%
80	11.459	3141	3147	3148	rBV	256	259	0.05%	0.006%
81	11.468	3148	3150	3152	rVV2	274	113	0.02%	0.003%
82	11.812	3244	3257	3273	rBV	276030	432037	85.33%	10.486%
83	11.886	3277	3280	3282	rBV	289	194	0.04%	0.005%
84	11.947	3294	3299	3303	rVB2	198	205	0.04%	0.005%
85	11.976	3303	3308	3315	rBV2	509	437	0.09%	0.011%
86	12.195	3363	3376	3392	rBV	237560	374799	74.03%	9.097%
87	12.767	3550	3554	3555	rBV	400	290	0.06%	0.007%
88	13.224	3693	3696	3707	rVB	254	253	0.05%	0.006%
89	13.661	3829	3832	3839	rVB	146	144	0.03%	0.003%
90	13.703	3839	3845	3848	rBV	132	151	0.03%	0.004%
91	14.160	3983	3987	3992	rBV	129	137	0.03%	0.003%
92	14.577	4112	4117	4127	rVB2	336	638	0.13%	0.015%
93	14.915	4218	4222	4226	rBV	175	150	0.03%	0.004%
94	15.166	4297	4300	4308	rVB2	257	245	0.05%	0.006%
95	15.346	4352	4356	4359	rBV	281	250	0.05%	0.006%
96	15.745	4478	4480	4483	rBV2	166	112	0.02%	0.003%
97	15.848	4509	4512	4513	rBV	227	135	0.03%	0.003%
98	16.018	4562	4565	4568	rBV	162	126	0.02%	0.003%
99	16.188	4614	4618	4621	rVB	422	251	0.05%	0.006%
100	16.532	4723	4725	4728	rVB2	364	163	0.03%	0.004%

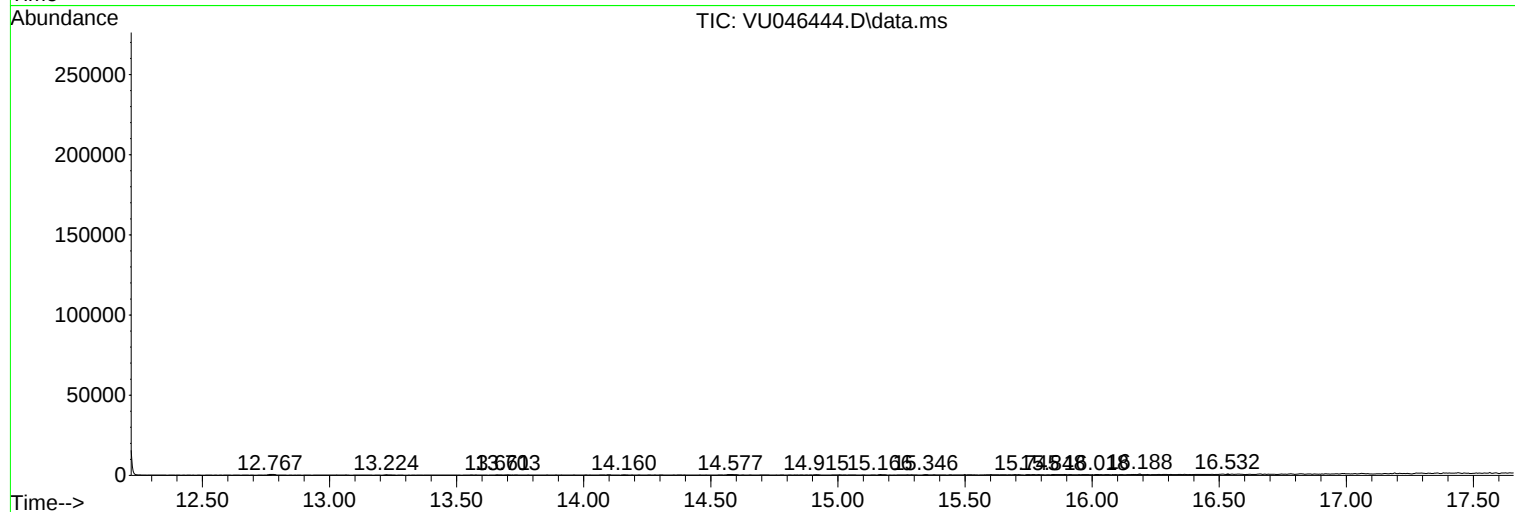
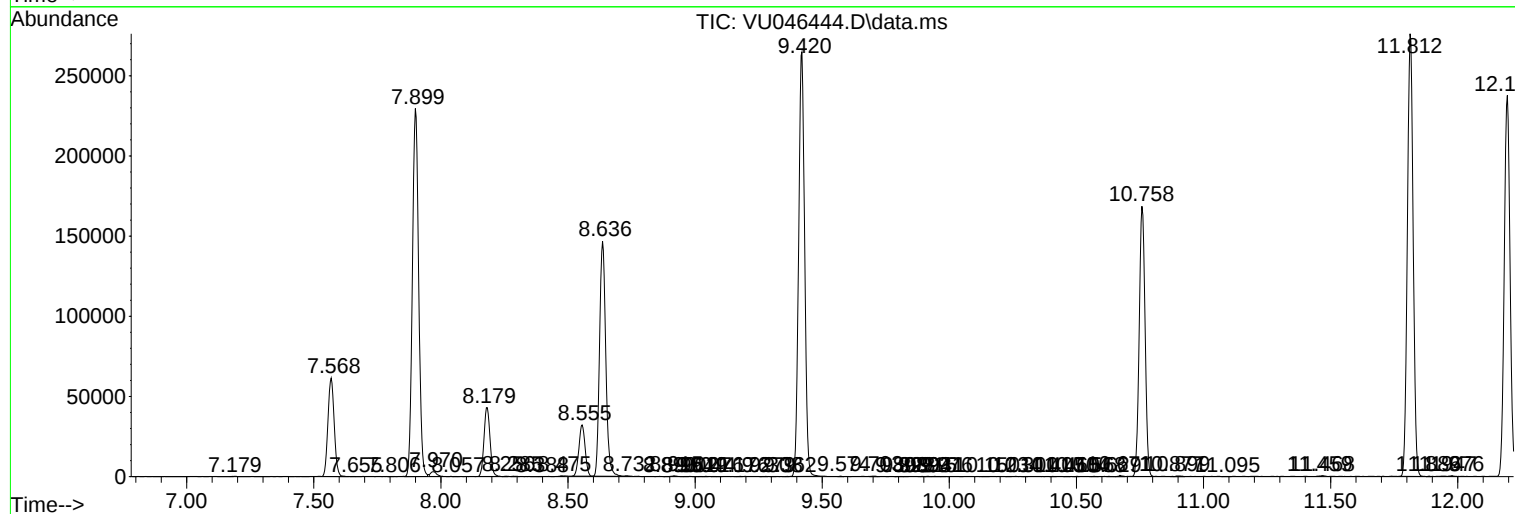
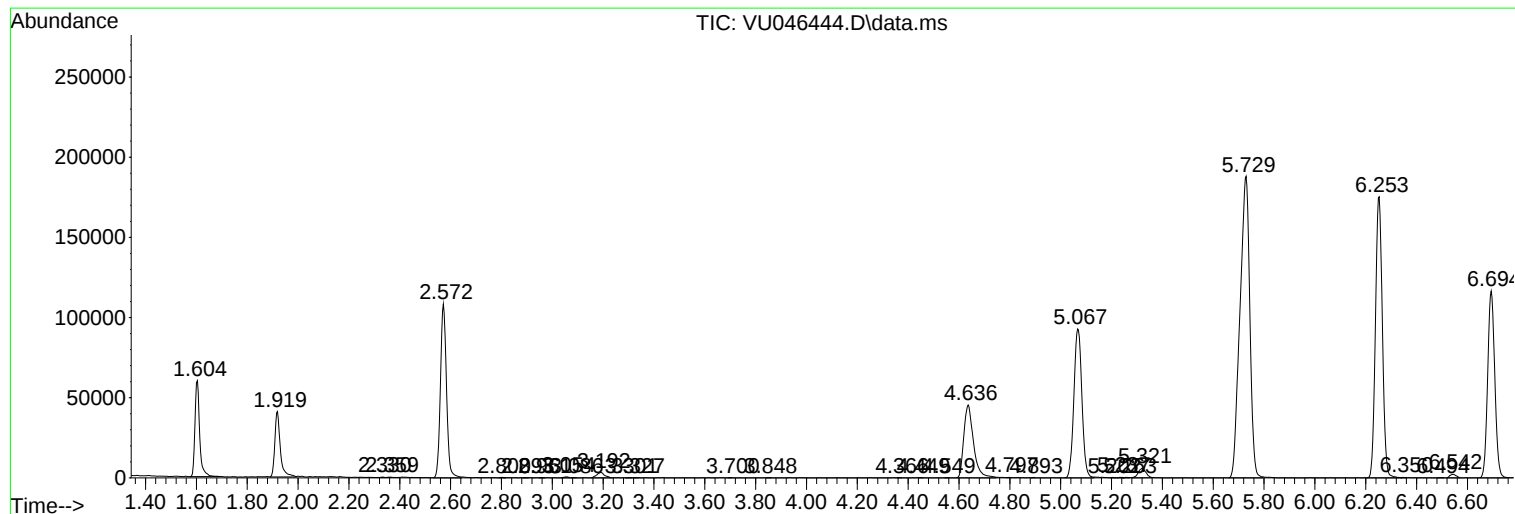
Sum of corrected areas: 4120045

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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



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TIC Library : C:\Database\NIST20.L
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No Library Search Compounds Detected

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