

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046456.D
 Acq On : 17 Dec 2021 05:19
 Operator : SY/MD
 Sample : M5121-11 20X
 Misc : 6.06g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL58

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: VU046456.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	74	82	99	rBV	60945	76019	14.53%	1.785%
2	1.919	172	180	201	rBV	41645	60130	11.49%	1.412%
3	2.571	372	383	402	rBV	109589	181233	34.64%	4.256%
4	2.787	447	450	452	rBV	176	138	0.03%	0.003%
5	2.848	467	469	470	rBV	250	120	0.02%	0.003%
6	2.909	485	488	491	rBV	156	157	0.03%	0.004%
7	2.973	505	508	511	rBB	157	129	0.02%	0.003%
8	3.115	549	552	555	rBB	155	134	0.03%	0.003%
9	3.144	559	561	563	rBV	126	90	0.02%	0.002%
10	3.192	563	576	593	rVB	7683	16896	3.23%	0.397%
11	3.343	620	623	626	rBB	144	121	0.02%	0.003%
12	3.411	642	644	647	rBB	137	93	0.02%	0.002%
13	3.523	677	679	682	rBV	141	125	0.02%	0.003%
14	3.575	693	695	697	rBV	133	99	0.02%	0.002%
15	3.687	727	730	734	rBB	159	155	0.03%	0.004%
16	3.793	759	763	765	rBB	137	111	0.02%	0.003%
17	4.632	1009	1024	1056	rBV2	49658	130595	24.96%	3.067%
18	4.861	1092	1095	1097	rBB	217	105	0.02%	0.002%
19	4.899	1101	1107	1109	rBV	126	178	0.03%	0.004%
20	4.970	1127	1129	1132	rBB	133	91	0.02%	0.002%
21	5.067	1141	1159	1186	rBV	95833	207401	39.65%	4.871%
22	5.176	1190	1193	1196	rVB	239	166	0.03%	0.004%
23	5.231	1206	1210	1213	rBV2	243	224	0.04%	0.005%
24	5.295	1228	1230	1233	rBB	137	96	0.02%	0.002%
25	5.362	1248	1251	1252	rBV	125	93	0.02%	0.002%
26	5.587	1319	1321	1323	rVB	237	94	0.02%	0.002%
27	5.729	1344	1365	1387	rBV2	193636	523142	100.00%	12.286%
28	5.944	1429	1432	1435	rBB	174	152	0.03%	0.004%
29	6.179	1503	1505	1510	rBB	129	137	0.03%	0.003%
30	6.250	1513	1527	1553	rBV	186471	349323	66.77%	8.204%
31	6.407	1572	1576	1579	rBB	139	146	0.03%	0.003%
32	6.530	1610	1614	1620	rBB3	477	456	0.09%	0.011%
33	6.558	1621	1623	1625	rBV	136	96	0.02%	0.002%
34	6.693	1651	1665	1687	rBV	119242	231560	44.26%	5.438%
35	6.809	1699	1701	1704	rBB	248	137	0.03%	0.003%
36	6.835	1704	1709	1711	rBB	151	152	0.03%	0.004%

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 Title : VOC Analysis

37	7.179	1813	1816	1820	rBV	191	238	0.05%	0.006%
38	7.275	1842	1846	1848	rBB	138	119	0.02%	0.003%
39	7.311	1854	1857	1861	rBB	140	120	0.02%	0.003%
40	7.465	1903	1905	1908	rBV	127	114	0.02%	0.003%
41	7.568	1925	1937	1952	rBV	62957	107455	20.54%	2.524%
42	7.665	1965	1967	1969	rBV	132	96	0.02%	0.002%
43	7.787	2001	2005	2011	rBB2	500	607	0.12%	0.014%
44	7.825	2014	2017	2019	rBV	136	121	0.02%	0.003%
45	7.899	2027	2040	2055	rBV	239287	409940	78.36%	9.627%
46	8.031	2078	2081	2084	rVB	229	150	0.03%	0.004%
47	8.076	2093	2095	2098	rBB	139	95	0.02%	0.002%
48	8.179	2116	2127	2144	rBV2	43143	71890	13.74%	1.688%
49	8.317	2167	2170	2172	rBV2	210	144	0.03%	0.003%
50	8.394	2189	2194	2196	rBB	148	150	0.03%	0.004%
51	8.484	2213	2222	2225	rBV2	520	787	0.15%	0.018%
52	8.636	2256	2269	2292	rBV	154354	258350	49.38%	6.067%
53	8.767	2307	2310	2316	rVB2	291	327	0.06%	0.008%
54	8.809	2320	2323	2326	rBV	155	152	0.03%	0.004%
55	8.877	2340	2344	2345	rBV	152	130	0.02%	0.003%
56	8.912	2349	2355	2363	rVV2	935	1443	0.28%	0.034%
57	9.015	2385	2387	2390	rBB	141	96	0.02%	0.002%
58	9.259	2459	2463	2465	rBB	138	112	0.02%	0.003%
59	9.295	2471	2474	2477	rBV	154	146	0.03%	0.003%
60	9.356	2491	2493	2497	rBB	154	102	0.02%	0.002%
61	9.420	2498	2513	2535	rBV	273430	452038	86.41%	10.616%
62	9.529	2545	2547	2550	rBB	139	97	0.02%	0.002%
63	9.565	2555	2558	2561	rBV2	227	180	0.03%	0.004%
64	9.668	2587	2590	2592	rBV	155	122	0.02%	0.003%
65	9.693	2594	2598	2604	rVV2	345	363	0.07%	0.009%
66	9.767	2617	2621	2626	rBB	153	203	0.04%	0.005%
67	9.857	2642	2649	2651	rBB	156	199	0.04%	0.005%
68	9.928	2669	2671	2673	rBV	141	104	0.02%	0.002%
69	10.105	2724	2726	2730	rBV	143	151	0.03%	0.004%
70	10.391	2813	2815	2817	rBV	133	93	0.02%	0.002%
71	10.471	2837	2840	2843	rBV	171	168	0.03%	0.004%
72	10.520	2853	2855	2858	rBB	131	91	0.02%	0.002%
73	10.542	2859	2862	2867	rBV	167	213	0.04%	0.005%
74	10.597	2877	2879	2882	rBB	143	96	0.02%	0.002%
75	10.626	2882	2888	2892	rBB	170	232	0.04%	0.005%
76	10.674	2895	2903	2909	rBV4	1276	1663	0.32%	0.039%

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77	10.758	2916	2929	2945	rVB	173729	274211	52.42%	6.440%
78	10.906	2971	2975	2979	rVB2	213	208	0.04%	0.005%
79	10.960	2989	2992	2994	rBB	156	108	0.02%	0.003%
80	10.999	3002	3004	3007	rBV	154	125	0.02%	0.003%
81	11.237	3074	3078	3081	rBV	172	204	0.04%	0.005%
82	11.381	3121	3123	3127	rVB	248	140	0.03%	0.003%
83	11.420	3130	3135	3139	rBV4	604	734	0.14%	0.017%
84	11.578	3178	3184	3187	rBV	525	625	0.12%	0.015%
85	11.693	3216	3220	3224	rBV	734	687	0.13%	0.016%
86	11.812	3245	3257	3275	rBV	315563	480767	91.90%	11.291%
87	11.976	3303	3308	3317	rVB4	1642	2112	0.40%	0.050%
88	12.031	3321	3325	3327	rBV	194	160	0.03%	0.004%
89	12.195	3363	3376	3395	rVB	255641	400361	76.53%	9.402%
90	12.430	3445	3449	3455	rBV	245	350	0.07%	0.008%
91	12.606	3501	3504	3508	rBV2	349	300	0.06%	0.007%
92	12.774	3549	3556	3563	rVB2	678	1026	0.20%	0.024%
93	12.819	3569	3570	3573	rBV	226	107	0.02%	0.003%
94	13.465	3768	3771	3775	rBV	391	252	0.05%	0.006%
95	13.584	3802	3808	3818	rVB4	1523	1865	0.36%	0.044%
96	14.192	3991	3997	4005	rBV3	1574	2330	0.45%	0.055%
97	14.635	4130	4135	4137	rBV	226	233	0.04%	0.005%
98	14.648	4137	4139	4143	rVB	546	330	0.06%	0.008%
99	15.015	4250	4253	4257	rBV	228	173	0.03%	0.004%
100	15.208	4308	4313	4315	rBV3	1684	1747	0.33%	0.041%

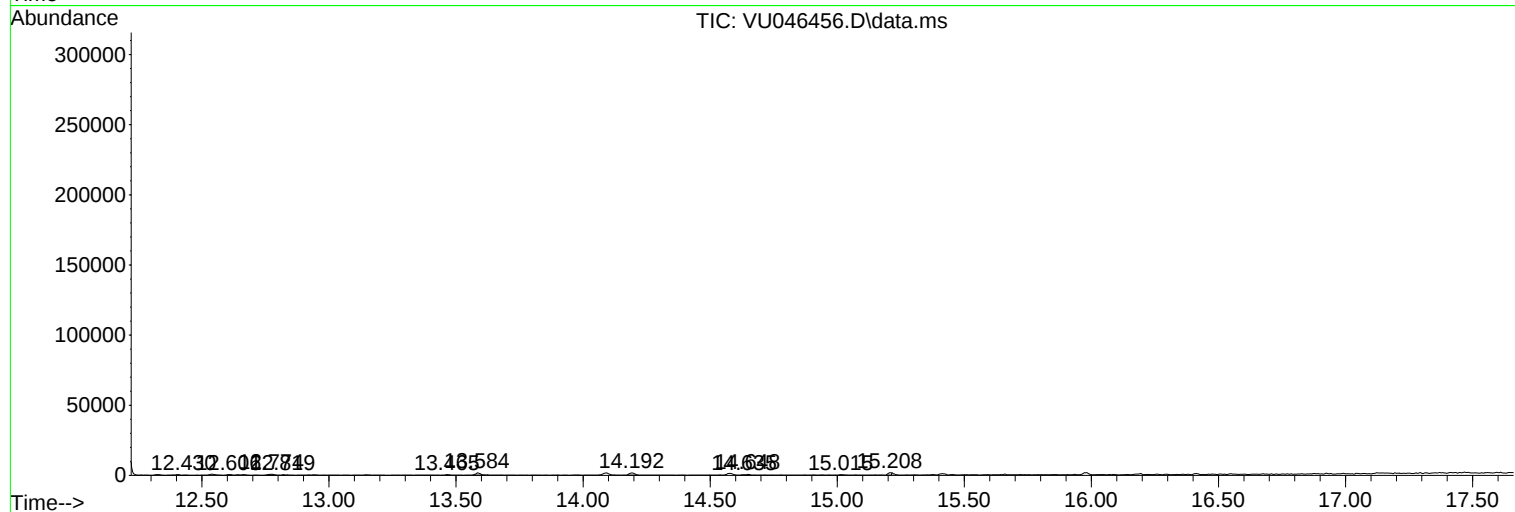
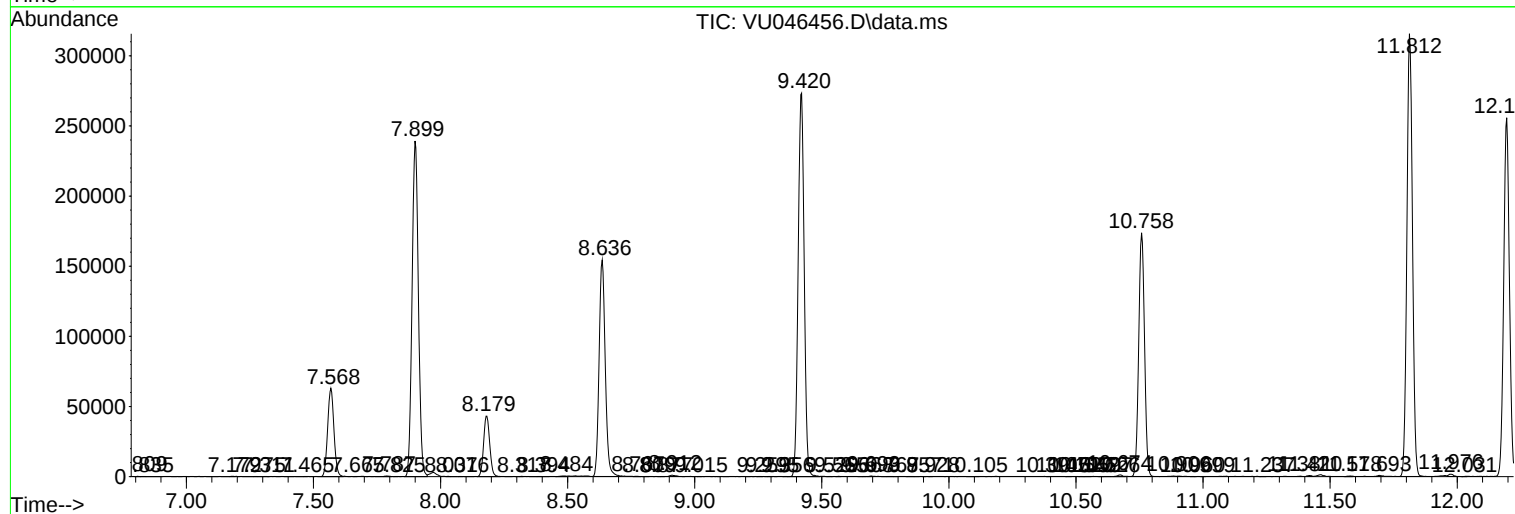
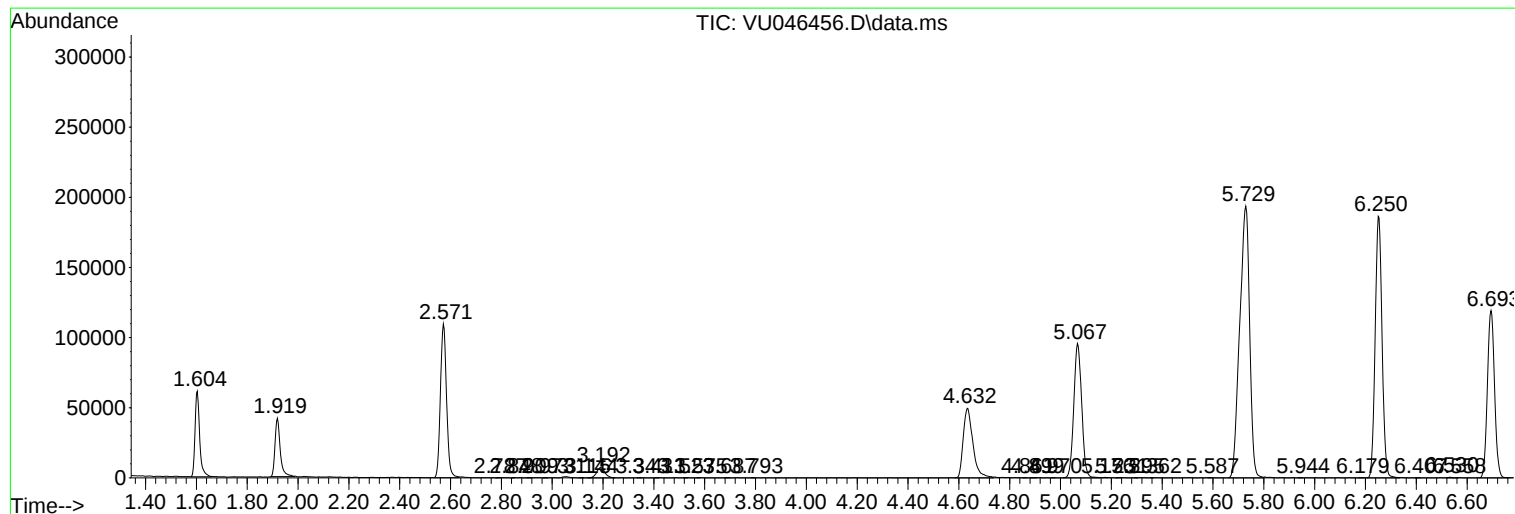
Sum of corrected areas: 4258146

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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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Quant Title : VOC Analysis

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

No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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