

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046449.D
 Acq On : 17 Dec 2021 02:41
 Operator : SY/MD
 Sample : M5121-03 20X
 Misc : 6.51g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL52

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: VU046449.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	100	rBV	58406	72219	14.89%	1.868%
2	1.919	171	180	198	rBV	41099	59410	12.25%	1.536%
3	2.353	309	315	319	rBV2	253	262	0.05%	0.007%
4	2.572	371	383	402	rBV	100276	165934	34.20%	4.291%
5	2.765	440	443	445	rBV	140	121	0.02%	0.003%
6	2.822	457	461	463	rBV	150	153	0.03%	0.004%
7	2.839	463	466	469	rVV	189	172	0.04%	0.004%
8	2.858	469	472	476	rVB	156	159	0.03%	0.004%
9	2.880	476	479	481	rBB	219	125	0.03%	0.003%
10	2.941	496	498	500	rVV	224	125	0.03%	0.003%
11	2.957	500	503	505	rVB	243	140	0.03%	0.004%
12	3.051	525	532	540	rBV3	1184	1942	0.40%	0.050%
13	3.186	562	574	592	rBV	8593	20235	4.17%	0.523%
14	3.440	651	653	658	rBB	156	157	0.03%	0.004%
15	3.498	668	671	674	rBB	129	119	0.02%	0.003%
16	3.713	735	738	741	rBV	161	152	0.03%	0.004%
17	4.636	1011	1025	1053	rBV	47895	126715	26.12%	3.277%
18	4.803	1074	1077	1082	rVV2	199	182	0.04%	0.005%
19	4.829	1082	1085	1088	rVB	260	186	0.04%	0.005%
20	4.973	1126	1130	1134	rBB	155	174	0.04%	0.004%
21	5.067	1144	1159	1179	rBV	90412	196344	40.47%	5.077%
22	5.244	1209	1214	1215	rBV	273	165	0.03%	0.004%
23	5.253	1215	1217	1220	rVV2	197	139	0.03%	0.004%
24	5.273	1220	1223	1227	rVV2	164	154	0.03%	0.004%
25	5.346	1243	1246	1250	rBB	271	219	0.05%	0.006%
26	5.639	1333	1337	1339	rBB	162	134	0.03%	0.003%
27	5.729	1344	1365	1385	rBV2	179848	485154	100.00%	12.546%
28	6.250	1514	1527	1549	rBV	163666	307315	63.34%	7.947%
29	6.533	1611	1615	1619	rBV2	460	415	0.09%	0.011%
30	6.607	1635	1638	1642	rBB	144	146	0.03%	0.004%
31	6.694	1651	1665	1685	rBB	114860	218209	44.98%	5.643%
32	6.813	1698	1702	1704	rBB	173	141	0.03%	0.004%
33	6.883	1721	1724	1728	rBV	122	156	0.03%	0.004%
34	7.047	1772	1775	1778	rBB	277	213	0.04%	0.006%
35	7.182	1814	1817	1819	rBV	178	146	0.03%	0.004%
36	7.568	1925	1937	1951	rBV2	57915	99830	20.58%	2.582%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.687	1972	1974	1977	rBV	270	156	0.03%	0.004%
38	7.761	1992	1997	1999	rBV	128	158	0.03%	0.004%
39	7.790	1999	2006	2008	rBV	652	781	0.16%	0.020%
40	7.899	2027	2040	2055	rBV	214745	364021	75.03%	9.414%
41	8.096	2098	2101	2104	rBV	174	164	0.03%	0.004%
42	8.137	2111	2114	2116	rBV	143	119	0.02%	0.003%
43	8.179	2116	2127	2140	rVV	41941	67671	13.95%	1.750%
44	8.240	2145	2146	2150	rVB2	316	167	0.03%	0.004%
45	8.481	2213	2221	2225	rBV	549	783	0.16%	0.020%
46	8.636	2256	2269	2298	rBV	144326	244889	50.48%	6.333%
47	8.768	2306	2310	2322	rVB2	344	727	0.15%	0.019%
48	8.819	2322	2326	2328	rBV	162	152	0.03%	0.004%
49	8.858	2336	2338	2343	rBB	155	153	0.03%	0.004%
50	8.915	2348	2356	2366	rBB3	1954	2974	0.61%	0.077%
51	9.022	2385	2389	2392	rBV	148	170	0.04%	0.004%
52	9.141	2424	2426	2429	rVV	171	141	0.03%	0.004%
53	9.218	2447	2450	2453	rBB	151	121	0.02%	0.003%
54	9.256	2460	2462	2467	rBV	150	186	0.04%	0.005%
55	9.350	2486	2491	2495	rBB	157	203	0.04%	0.005%
56	9.420	2498	2513	2534	rBV	243636	398077	82.05%	10.294%
57	9.507	2537	2540	2543	rBV	252	209	0.04%	0.005%
58	9.629	2575	2578	2580	rBV	145	122	0.03%	0.003%
59	9.668	2584	2590	2592	rBV	150	209	0.04%	0.005%
60	9.687	2593	2596	2601	rVB2	344	350	0.07%	0.009%
61	9.919	2664	2668	2671	rBB	162	128	0.03%	0.003%
62	10.022	2698	2700	2703	rBV	173	134	0.03%	0.003%
63	10.153	2737	2741	2746	rVB	204	258	0.05%	0.007%
64	10.282	2777	2781	2784	rVB	204	186	0.04%	0.005%
65	10.427	2823	2826	2828	rBB	191	119	0.02%	0.003%
66	10.449	2829	2833	2835	rBV	166	147	0.03%	0.004%
67	10.552	2861	2865	2868	rVB	210	186	0.04%	0.005%
68	10.600	2876	2880	2886	rBB	155	221	0.05%	0.006%
69	10.639	2887	2892	2896	rBB	192	227	0.05%	0.006%
70	10.671	2896	2902	2908	rBV	734	891	0.18%	0.023%
71	10.758	2916	2929	2944	rBV	165532	260204	53.63%	6.729%
72	10.877	2962	2966	2967	rBV	156	129	0.03%	0.003%
73	10.899	2971	2973	2975	rVV	193	121	0.02%	0.003%
74	11.414	3126	3133	3138	rBB	197	315	0.06%	0.008%
75	11.452	3139	3145	3148	rBV2	429	583	0.12%	0.015%
76	11.555	3175	3177	3180	rBV	155	125	0.03%	0.003%

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77	11.726	3227	3230	3232	rBV	204	169	0.03%	0.004%
78	11.812	3245	3257	3274	rVB	260802	404664	83.41%	10.465%
79	11.938	3293	3296	3298	rBV	208	142	0.03%	0.004%
80	11.976	3303	3308	3313	rVB2	416	526	0.11%	0.014%
81	12.195	3364	3376	3393	rBV	222902	351927	72.54%	9.101%
82	12.771	3550	3555	3566	rVB2	646	1009	0.21%	0.026%
83	13.150	3668	3673	3676	rBV	147	163	0.03%	0.004%
84	13.571	3801	3804	3810	rVB	144	140	0.03%	0.004%
85	14.092	3963	3966	3970	rBV	178	173	0.04%	0.004%
86	14.578	4109	4117	4127	rVB	665	1041	0.21%	0.027%
87	15.365	4359	4362	4365	rBV2	211	122	0.03%	0.003%
88	15.471	4391	4395	4397	rBV	185	160	0.03%	0.004%
89	15.552	4418	4420	4425	rBV2	184	201	0.04%	0.005%
90	15.767	4484	4487	4491	rBV	251	257	0.05%	0.007%
91	15.825	4502	4505	4507	rBV	209	162	0.03%	0.004%
92	16.034	4567	4570	4572	rBV	231	156	0.03%	0.004%
93	16.095	4586	4589	4592	rBV2	295	213	0.04%	0.006%
94	16.134	4598	4601	4605	rBV2	198	192	0.04%	0.005%
95	16.269	4640	4643	4647	rBV2	238	156	0.03%	0.004%
96	16.674	4767	4769	4772	rBV2	247	153	0.03%	0.004%
97	16.770	4797	4799	4802	rBV	346	196	0.04%	0.005%
98	17.253	4946	4949	4953	rBV3	541	392	0.08%	0.010%
99	17.272	4953	4955	4957	rBV	351	145	0.03%	0.004%
100	17.336	4973	4975	4978	rBV2	436	280	0.06%	0.007%

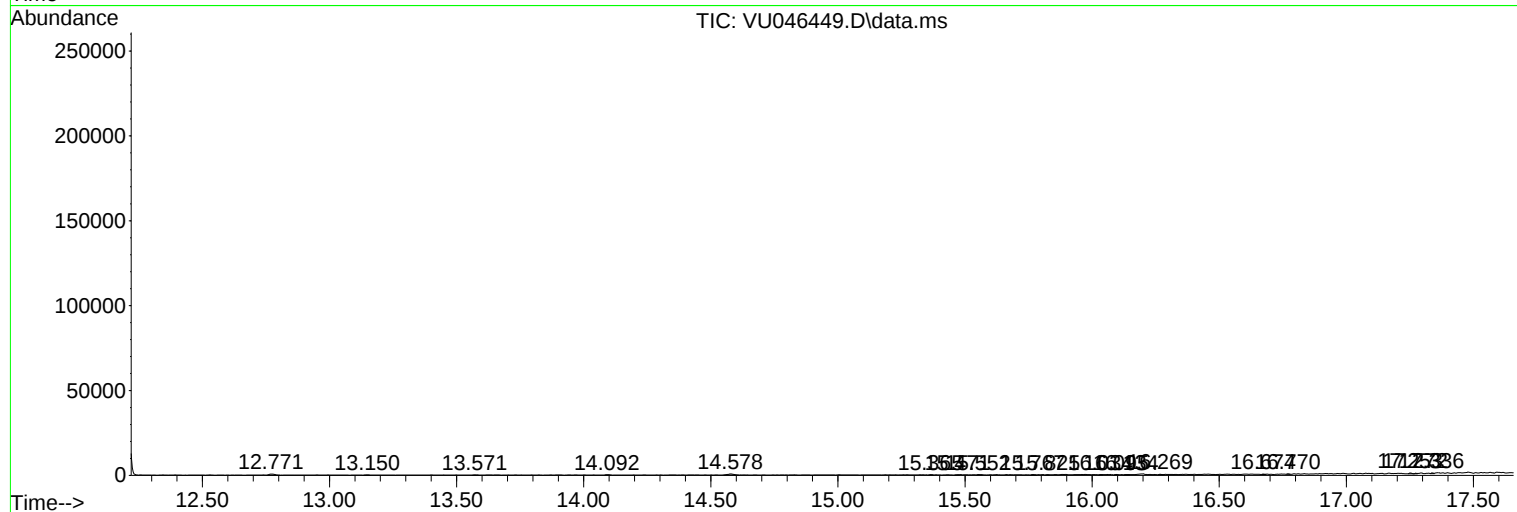
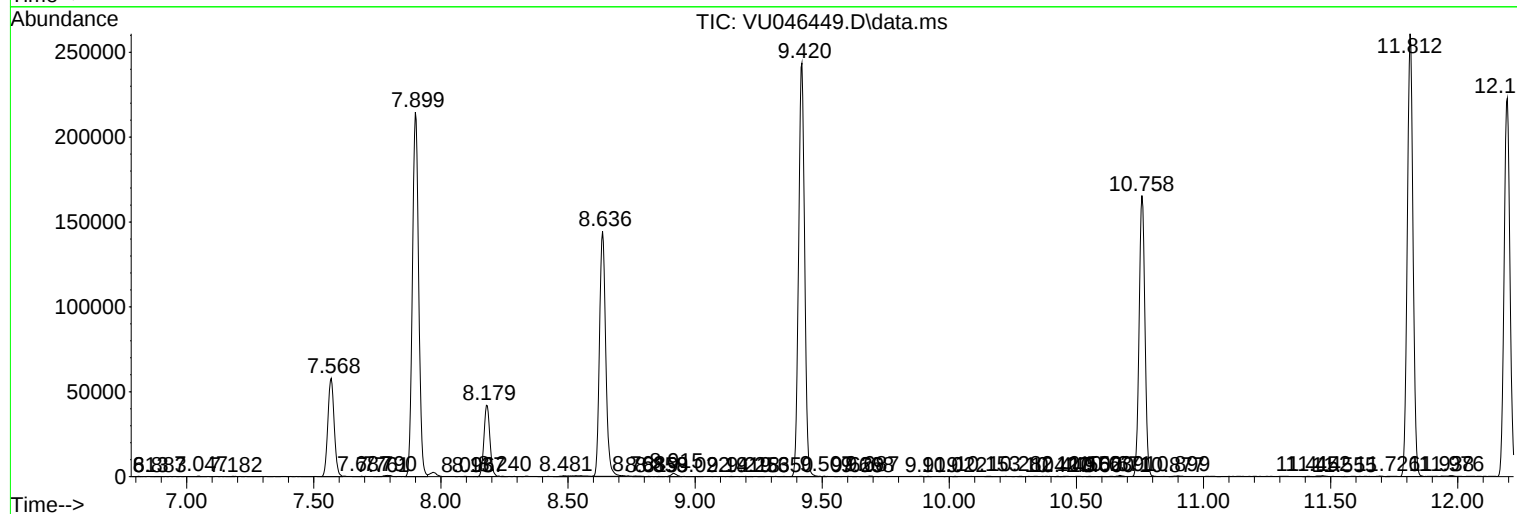
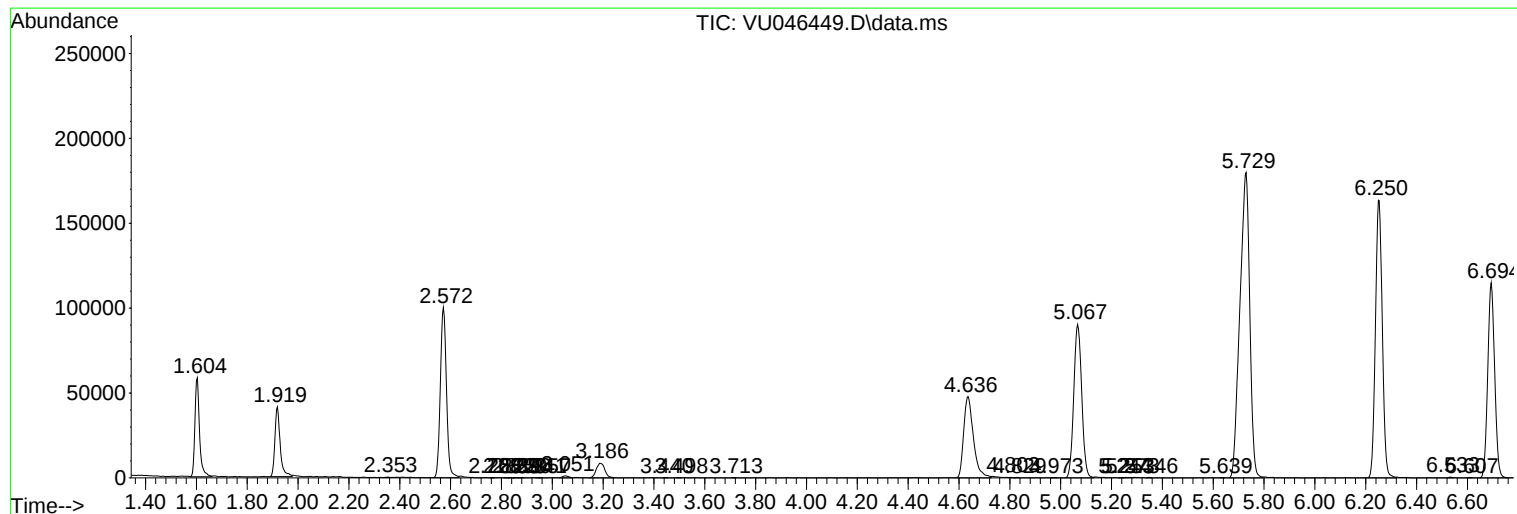
Sum of corrected areas: 3866978

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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	--Internal Standard--			
					#	RT	Resp	Conc