

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121621\
 Data File : VU046440.D
 Acq On : 16 Dec 2021 23:17
 Operator : SY/MD
 Sample : M5101-12ME
 Misc : 6.90g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL36ME

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: VU046440.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	72	81	112	rVB	38030	76206	14.79%	1.561%
2	1.858	158	161	164	rBV3	547	495	0.10%	0.010%
3	1.916	170	179	209	rBV	21765	56669	11.00%	1.160%
4	2.543	363	374	393	rBV	84002	157996	30.66%	3.235%
5	3.041	520	529	539	rVB5	1225	2201	0.43%	0.045%
6	3.090	540	544	547	rBV	143	143	0.03%	0.003%
7	3.109	547	550	557	rVB	180	244	0.05%	0.005%
8	3.183	558	573	590	rBV2	12770	31211	6.06%	0.639%
9	3.331	617	619	623	rVB2	361	279	0.05%	0.006%
10	3.360	624	628	631	rVB2	216	186	0.04%	0.004%
11	3.382	631	635	637	rBV2	192	176	0.03%	0.004%
12	3.565	689	692	696	rBV	130	164	0.03%	0.003%
13	3.787	758	761	764	rBV	172	163	0.03%	0.003%
14	3.861	772	784	798	rVB2	3783	8769	1.70%	0.180%
15	4.559	999	1001	1007	rBV	138	182	0.04%	0.004%
16	4.659	1016	1032	1056	rBV2	26532	109542	21.26%	2.243%
17	4.906	1106	1109	1112	rBV	294	216	0.04%	0.004%
18	5.064	1139	1158	1179	rBV	87008	203185	39.43%	4.161%
19	5.311	1218	1235	1256	rBV	96982	218976	42.50%	4.484%
20	5.398	1259	1262	1265	rBV	224	177	0.03%	0.004%
21	5.720	1343	1362	1384	rBV2	203236	515253	100.00%	10.551%
22	5.819	1391	1393	1396	rBB	255	145	0.03%	0.003%
23	5.874	1407	1410	1414	rBB	135	142	0.03%	0.003%
24	5.987	1433	1445	1465	rBB7	3436	9192	1.78%	0.188%
25	6.138	1488	1492	1495	rBB	137	140	0.03%	0.003%
26	6.250	1512	1527	1552	rVV	178327	354944	68.89%	7.269%
27	6.337	1552	1554	1558	rVB2	308	247	0.05%	0.005%
28	6.543	1605	1618	1630	rBV2	16952	32884	6.38%	0.673%
29	6.604	1630	1637	1639	rBV3	1302	1516	0.29%	0.031%
30	6.694	1650	1665	1688	rVB	111778	229531	44.55%	4.700%
31	7.115	1792	1796	1799	rBB	155	154	0.03%	0.003%
32	7.189	1815	1819	1822	rBV2	272	282	0.05%	0.006%
33	7.218	1826	1828	1830	rVV	418	288	0.06%	0.006%
34	7.231	1830	1832	1834	rVV2	544	346	0.07%	0.007%
35	7.244	1834	1836	1840	rVV	406	322	0.06%	0.007%
36	7.260	1840	1841	1843	rVV	382	171	0.03%	0.004%

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

37	7.569	1925	1937	1959	rVV	55656	111165	21.57%	2.276%
38	7.675	1967	1970	1976	rBV	148	208	0.04%	0.004%
39	7.797	1996	2008	2021	rBB4	2266	4283	0.83%	0.088%
40	7.900	2027	2040	2056	rBV	227279	405973	78.79%	8.314%
41	7.974	2056	2063	2071	rVV3	3541	5071	0.98%	0.104%
42	8.067	2090	2092	2095	rVB	363	163	0.03%	0.003%
43	8.186	2117	2129	2154	rBV3	31286	75341	14.62%	1.543%
44	8.459	2210	2214	2215	rBV	240	163	0.03%	0.003%
45	8.472	2215	2218	2220	rVV2	461	353	0.07%	0.007%
46	8.501	2221	2227	2231	rVV3	735	1159	0.22%	0.024%
47	8.552	2231	2243	2259	rVB	236825	405401	78.68%	8.302%
48	8.684	2261	2284	2310	rBV	88691	253053	49.11%	5.182%
49	8.797	2315	2319	2321	rVB2	301	201	0.04%	0.004%
50	8.913	2351	2355	2359	rBV	140	193	0.04%	0.004%
51	8.954	2362	2368	2370	rVV	619	651	0.13%	0.013%
52	9.015	2385	2387	2394	rBB	154	179	0.03%	0.004%
53	9.224	2448	2452	2455	rBB	155	146	0.03%	0.003%
54	9.424	2500	2514	2534	rBV	223439	473750	91.95%	9.702%
55	9.578	2556	2562	2567	rBV2	353	539	0.10%	0.011%
56	9.658	2580	2587	2589	rBB	145	168	0.03%	0.003%
57	9.700	2594	2600	2607	rBV2	567	918	0.18%	0.019%
58	9.810	2631	2634	2637	rBV	131	138	0.03%	0.003%
59	9.951	2675	2678	2681	rBV	166	157	0.03%	0.003%
60	10.109	2724	2727	2729	rBV2	257	187	0.04%	0.004%
61	10.366	2804	2807	2810	rBV	161	163	0.03%	0.003%
62	10.382	2810	2812	2816	rVB	198	157	0.03%	0.003%
63	10.411	2817	2821	2826	rBV	168	238	0.05%	0.005%
64	10.675	2897	2903	2910	rBV3	1109	1501	0.29%	0.031%
65	10.774	2921	2934	2948	rVB	166543	270730	52.54%	5.544%
66	10.900	2966	2973	2975	rBV2	474	470	0.09%	0.010%
67	11.118	3037	3041	3046	rBV2	873	727	0.14%	0.015%
68	11.337	3104	3109	3113	rVB	205	260	0.05%	0.005%
69	11.363	3114	3117	3120	rBV	157	150	0.03%	0.003%
70	11.459	3142	3147	3148	rBV	477	383	0.07%	0.008%
71	11.533	3167	3170	3171	rBV	215	144	0.03%	0.003%
72	11.575	3179	3183	3188	rBV2	186	153	0.03%	0.003%
73	11.617	3193	3196	3198	rBV	157	139	0.03%	0.003%
74	11.700	3219	3222	3225	rVB	305	221	0.04%	0.005%
75	11.752	3235	3238	3243	rBV2	509	564	0.11%	0.012%
76	11.819	3246	3259	3276	rVB	301609	474164	92.03%	9.710%

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77	11.938	3293	3296	3299	rVB	284	177	0.03%	0.004%
78	11.977	3299	3308	3312	rBV2	559	635	0.12%	0.013%
79	12.202	3364	3378	3393	rVV	230456	372683	72.33%	7.632%
80	12.469	3457	3461	3464	rVV	146	143	0.03%	0.003%
81	12.777	3550	3557	3562	rVB	664	909	0.18%	0.019%
82	13.109	3655	3660	3665	rVB	140	149	0.03%	0.003%
83	13.227	3694	3697	3703	rVB2	426	490	0.10%	0.010%
84	13.851	3885	3891	3895	rVB2	357	490	0.10%	0.010%
85	14.092	3960	3966	3974	rBV2	431	576	0.11%	0.012%
86	14.330	4037	4040	4043	rBV3	351	273	0.05%	0.006%
87	14.578	4110	4117	4124	rVB	727	1190	0.23%	0.024%
88	15.337	4348	4353	4356	rVB2	185	169	0.03%	0.003%
89	15.497	4400	4403	4408	rVV2	179	147	0.03%	0.003%
90	15.562	4420	4423	4427	rBV	232	154	0.03%	0.003%
91	15.604	4431	4436	4439	rBV	156	168	0.03%	0.003%
92	15.678	4452	4459	4463	rBV2	216	302	0.06%	0.006%
93	15.755	4479	4483	4486	rBV2	232	225	0.04%	0.005%
94	15.800	4490	4497	4501	rBV2	257	390	0.08%	0.008%
95	15.825	4501	4505	4509	rBV2	239	227	0.04%	0.005%
96	16.034	4567	4570	4573	rVB2	258	142	0.03%	0.003%
97	16.317	4655	4658	4663	rBV2	263	268	0.05%	0.005%
98	16.414	4685	4688	4695	rVB	264	180	0.03%	0.004%
99	16.552	4727	4731	4733	rBV	381	304	0.06%	0.006%
100	16.890	4833	4836	4841	rVB3	529	373	0.07%	0.008%

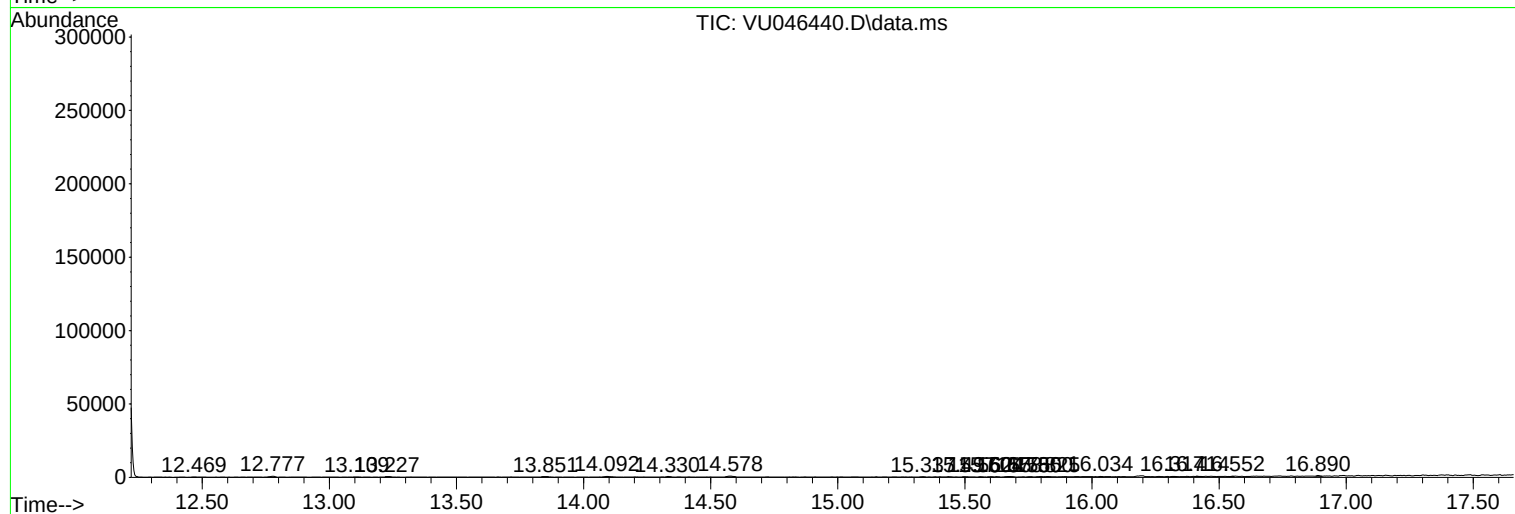
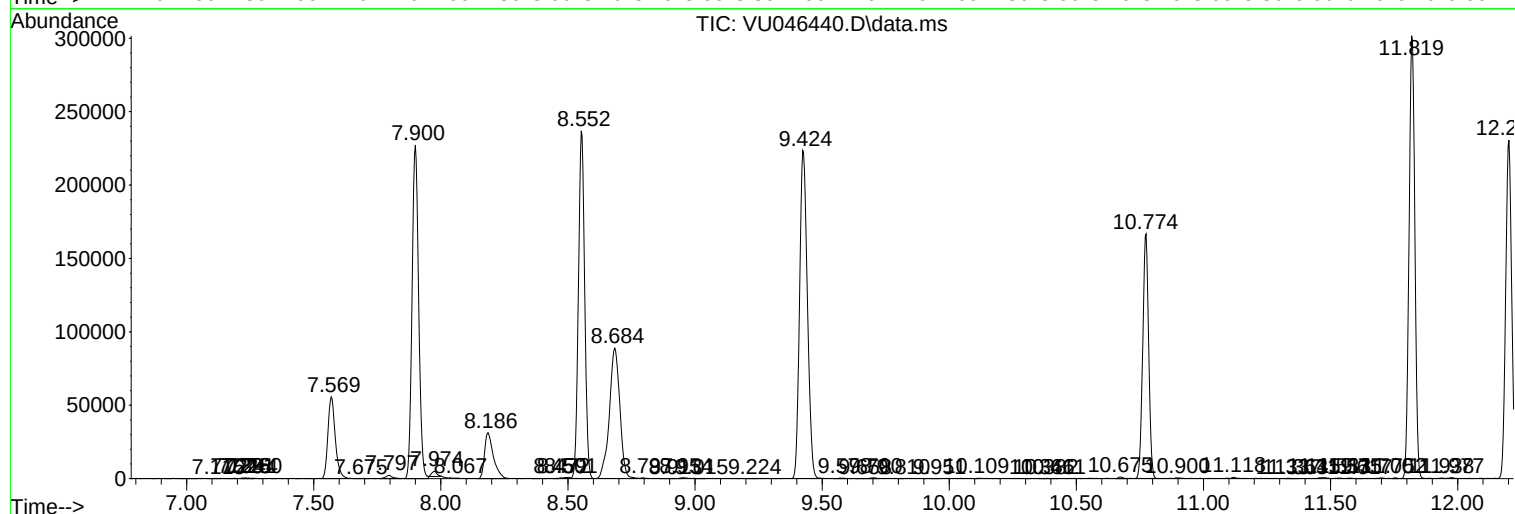
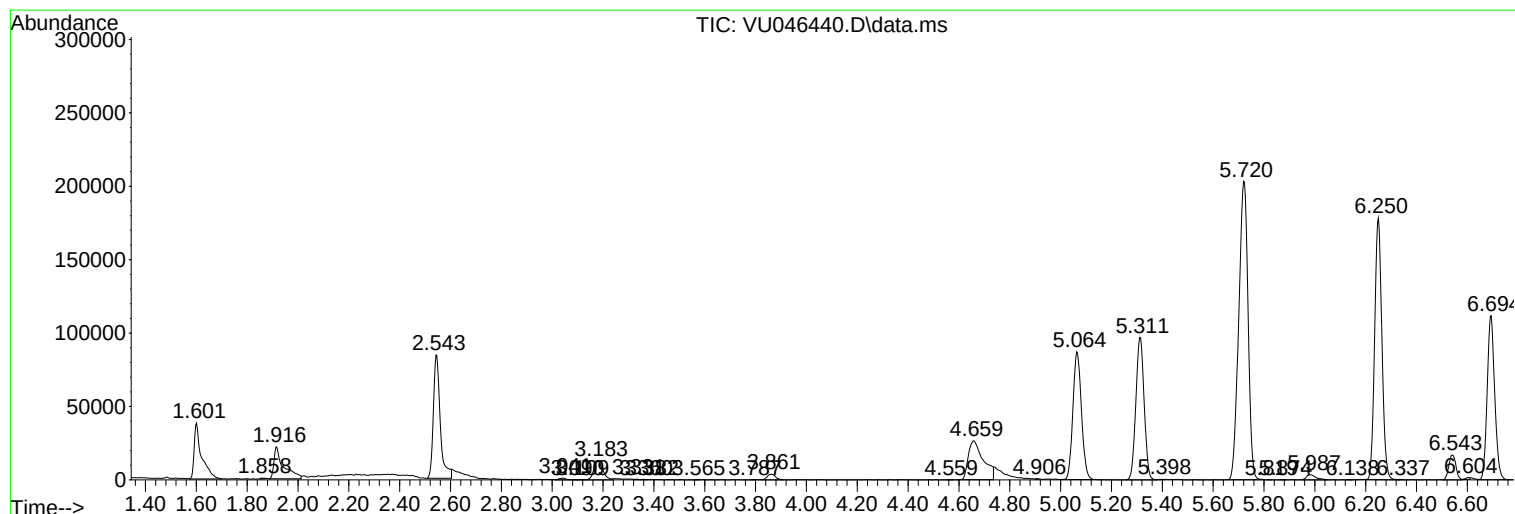
Sum of corrected areas: 4883225

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BGL36ME

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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MSVOA_U
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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

No Library Search Compounds Detected

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