

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120921\
 Data File : VU046211.D
 Acq On : 09 Dec 2021 11:49
 Operator : SY/MD
 Sample : M4960-01ME
 Misc : 6.06g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKR4ME

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: VU046211.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	74	81	95	rVB	91726	118623	11.77%	1.402%
2	1.919	173	180	202	rVB	60999	103678	10.29%	1.226%
3	2.076	227	229	233	rVB	569	355	0.04%	0.004%
4	2.205	262	269	271	rBV5	901	833	0.08%	0.010%
5	2.231	272	277	279	rBV4	350	320	0.03%	0.004%
6	2.295	294	297	300	rBV4	621	421	0.04%	0.005%
7	2.314	300	303	308	rBV5	478	576	0.06%	0.007%
8	2.511	361	364	365	rBV3	663	376	0.04%	0.004%
9	2.552	365	377	391	rVV	127084	204430	20.28%	2.417%
10	2.855	468	471	477	rVB5	737	689	0.07%	0.008%
11	2.887	477	481	486	rBV3	599	644	0.06%	0.008%
12	3.041	519	529	544	rVB4	6610	13282	1.32%	0.157%
13	3.186	562	574	586	rBV	4088	9338	0.93%	0.110%
14	3.433	644	651	653	rBV3	463	505	0.05%	0.006%
15	3.761	746	753	755	rBV	483	586	0.06%	0.007%
16	4.009	827	830	837	rVB	395	392	0.04%	0.005%
17	4.166	874	879	882	rBV	390	405	0.04%	0.005%
18	4.244	898	903	908	rBV2	437	483	0.05%	0.006%
19	4.408	950	954	959	rBV2	397	413	0.04%	0.005%
20	4.658	1015	1032	1079	rBV2	56684	265923	26.38%	3.144%
21	5.067	1143	1159	1191	rVB4	151862	402253	39.90%	4.755%
22	5.195	1191	1199	1203	rBV	508	653	0.06%	0.008%
23	5.234	1207	1211	1217	rBV	489	410	0.04%	0.005%
24	5.469	1280	1284	1286	rBV	511	353	0.04%	0.004%
25	5.723	1342	1363	1392	rBV2	378811	973935	96.62%	11.513%
26	5.829	1392	1396	1400	rBV3	652	559	0.06%	0.007%
27	5.983	1434	1444	1460	rBV5	4546	11980	1.19%	0.142%
28	6.192	1503	1509	1512	rBV	379	436	0.04%	0.005%
29	6.250	1512	1527	1552	rVV	262665	538832	53.45%	6.370%
30	6.533	1605	1615	1628	rBV5	4885	11020	1.09%	0.130%
31	6.597	1633	1635	1638	rBV2	717	492	0.05%	0.006%
32	6.694	1651	1665	1686	rBV	216043	442374	43.89%	5.229%
33	6.803	1694	1699	1701	rBV	608	616	0.06%	0.007%
34	7.015	1762	1765	1770	rVB	493	401	0.04%	0.005%
35	7.189	1814	1819	1823	rBV2	488	498	0.05%	0.006%
36	7.382	1875	1879	1884	rBV2	489	487	0.05%	0.006%

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

37	7.568	1924	1937	1966	rBV	122633	246296	24.43%	2.912%
38	7.793	1998	2007	2015	rBV5	2220	3883	0.39%	0.046%
39	7.899	2026	2040	2059	rBV	423926	798597	79.22%	9.441%
40	8.054	2085	2088	2094	rVB2	678	609	0.06%	0.007%
41	8.131	2108	2112	2115	rBV2	624	466	0.05%	0.006%
42	8.186	2115	2129	2156	rVV	72551	168430	16.71%	1.991%
43	8.475	2213	2219	2225	rBV3	685	960	0.10%	0.011%
44	8.555	2232	2244	2259	rVB2	94529	163011	16.17%	1.927%
45	8.690	2260	2286	2319	rVV2	178573	565713	56.12%	6.688%
46	8.951	2364	2367	2372	rBV3	482	507	0.05%	0.006%
47	9.224	2448	2452	2458	rVB2	308	423	0.04%	0.005%
48	9.427	2500	2515	2539	rBV	302504	713449	70.78%	8.434%
49	9.568	2555	2559	2564	rBV5	708	727	0.07%	0.009%
50	9.671	2588	2591	2593	rBV	532	349	0.03%	0.004%
51	9.703	2593	2601	2606	rVV5	1410	2360	0.23%	0.028%
52	9.922	2666	2669	2673	rVB	558	464	0.05%	0.005%
53	10.468	2835	2839	2844	rBV2	661	564	0.06%	0.007%
54	10.613	2881	2884	2888	rBV2	389	409	0.04%	0.005%
55	10.674	2894	2903	2914	rVB3	3853	5743	0.57%	0.068%
56	10.722	2914	2918	2921	rBV	508	459	0.05%	0.005%
57	10.774	2921	2934	2957	rBV	344390	580215	57.56%	6.859%
58	10.870	2961	2964	2965	rBV2	463	318	0.03%	0.004%
59	11.025	3008	3012	3020	rVB2	455	647	0.06%	0.008%
60	11.115	3033	3040	3048	rVB6	2231	3509	0.35%	0.041%
61	11.320	3102	3104	3110	rVB	673	507	0.05%	0.006%
62	11.353	3110	3114	3117	rBV2	691	597	0.06%	0.007%
63	11.459	3140	3147	3161	rVB5	3290	6709	0.67%	0.079%
64	11.546	3170	3174	3179	rVB	439	427	0.04%	0.005%
65	11.584	3179	3186	3194	rBV2	1234	1663	0.16%	0.020%
66	11.642	3201	3204	3209	rBV3	343	328	0.03%	0.004%
67	11.700	3214	3222	3235	rBV4	3548	5928	0.59%	0.070%
68	11.755	3235	3239	3247	rBV4	889	1034	0.10%	0.012%
69	11.822	3247	3260	3280	rBV2	493775	1008029	100.00%	11.916%
70	11.947	3292	3299	3302	rBV3	1995	2716	0.27%	0.032%
71	12.201	3361	3378	3394	rVB	502419	804639	79.82%	9.512%
72	12.330	3410	3418	3426	rVB4	4478	6335	0.63%	0.075%
73	12.401	3437	3440	3443	rVV4	1015	664	0.07%	0.008%
74	12.462	3455	3459	3462	rBV	456	398	0.04%	0.005%
75	12.591	3497	3499	3506	rBV3	324	358	0.04%	0.004%
76	12.864	3578	3584	3588	rVB	540	702	0.07%	0.008%

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 Title : VOC Analysis

77	12.918	3598	3601	3609	rVV	399	505	0.05%	0.006%
78	13.041	3631	3639	3640	rBV2	642	821	0.08%	0.010%
79	13.140	3667	3670	3676	rBV3	682	853	0.08%	0.010%
80	13.230	3695	3698	3703	rVB2	851	742	0.07%	0.009%
81	13.269	3707	3710	3715	rVB	642	508	0.05%	0.006%
82	13.433	3757	3761	3766	rVB4	1339	1134	0.11%	0.013%
83	13.520	3783	3788	3794	rBV2	460	578	0.06%	0.007%
84	13.584	3805	3808	3811	rVB2	500	318	0.03%	0.004%
85	13.754	3856	3861	3863	rBV	399	343	0.03%	0.004%
86	13.845	3880	3889	3896	rBV3	1815	2648	0.26%	0.031%
87	14.089	3953	3965	3980	rBV	107001	165860	16.45%	1.961%
88	14.221	4000	4006	4009	rBV3	508	639	0.06%	0.008%
89	14.291	4025	4028	4033	rVV3	534	542	0.05%	0.006%
90	14.336	4033	4042	4049	rVB3	1263	1951	0.19%	0.023%
91	14.452	4074	4078	4083	rVB2	1272	1128	0.11%	0.013%
92	14.861	4198	4205	4208	rBV3	883	1020	0.10%	0.012%
93	15.224	4310	4318	4330	rVB	10992	15791	1.57%	0.187%
94	15.410	4361	4376	4386	rBV3	9231	14948	1.48%	0.177%
95	15.590	4429	4432	4434	rBV	449	315	0.03%	0.004%
96	15.954	4538	4545	4556	rVB3	2859	4429	0.44%	0.052%
97	16.073	4579	4582	4586	rBV2	585	567	0.06%	0.007%
98	16.262	4633	4641	4650	rBV5	2912	4834	0.48%	0.057%
99	16.410	4680	4687	4694	rBV3	5602	7818	0.78%	0.092%
100	17.098	4893	4901	4913	rVB	14632	24225	2.40%	0.286%

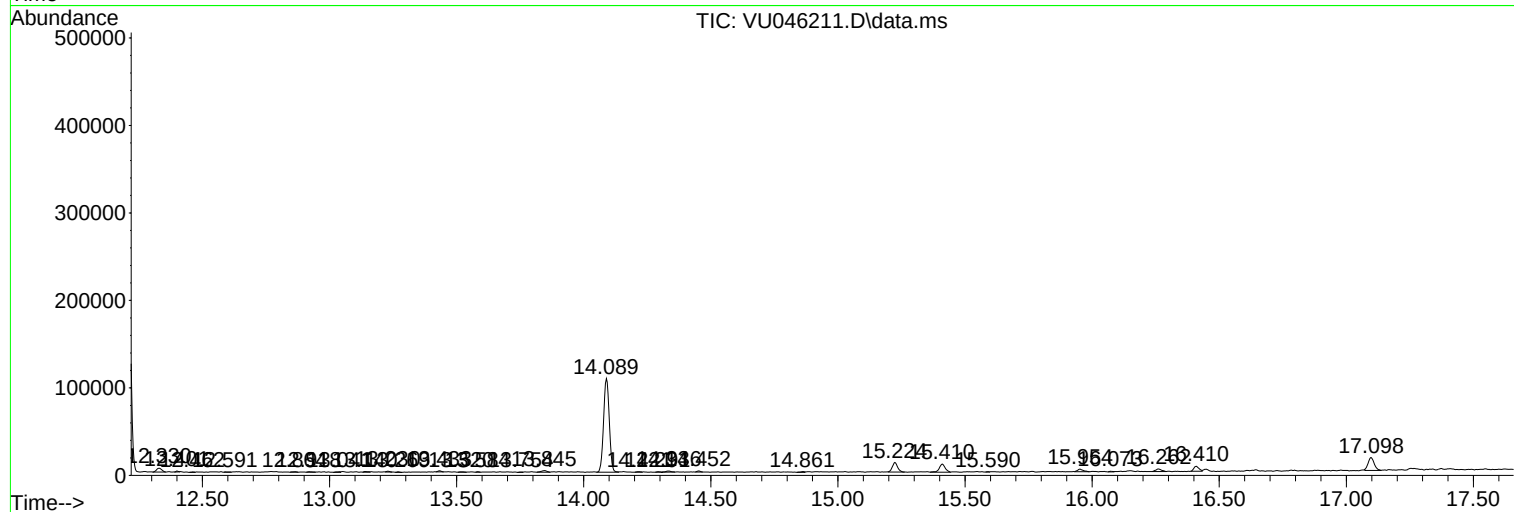
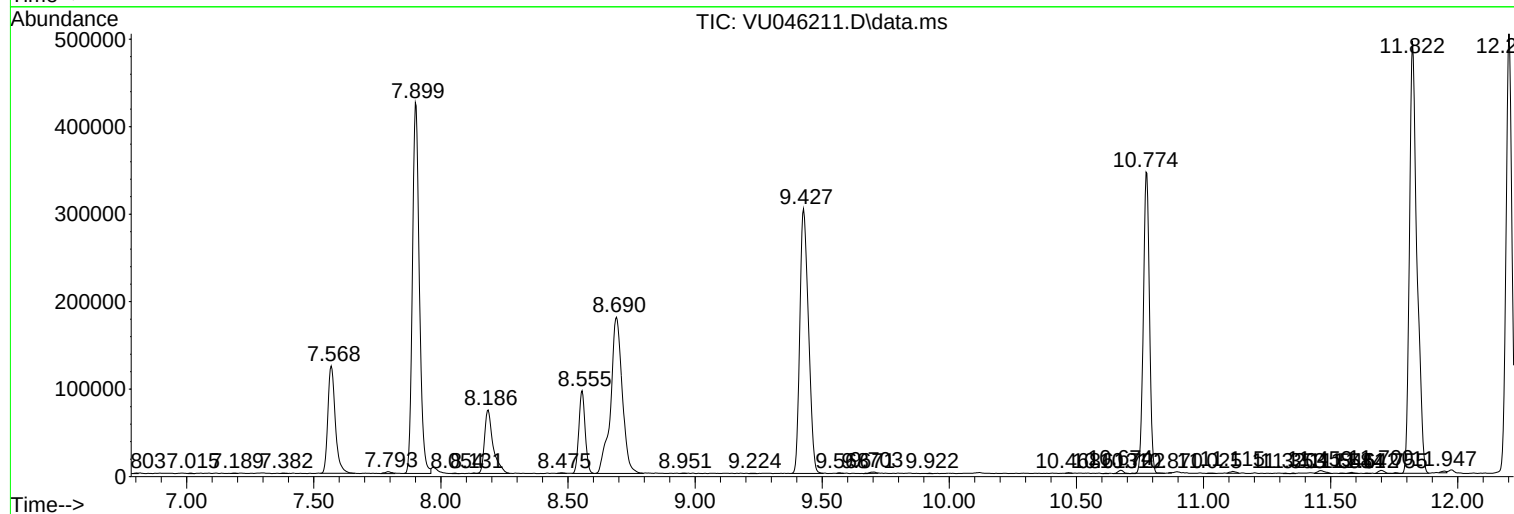
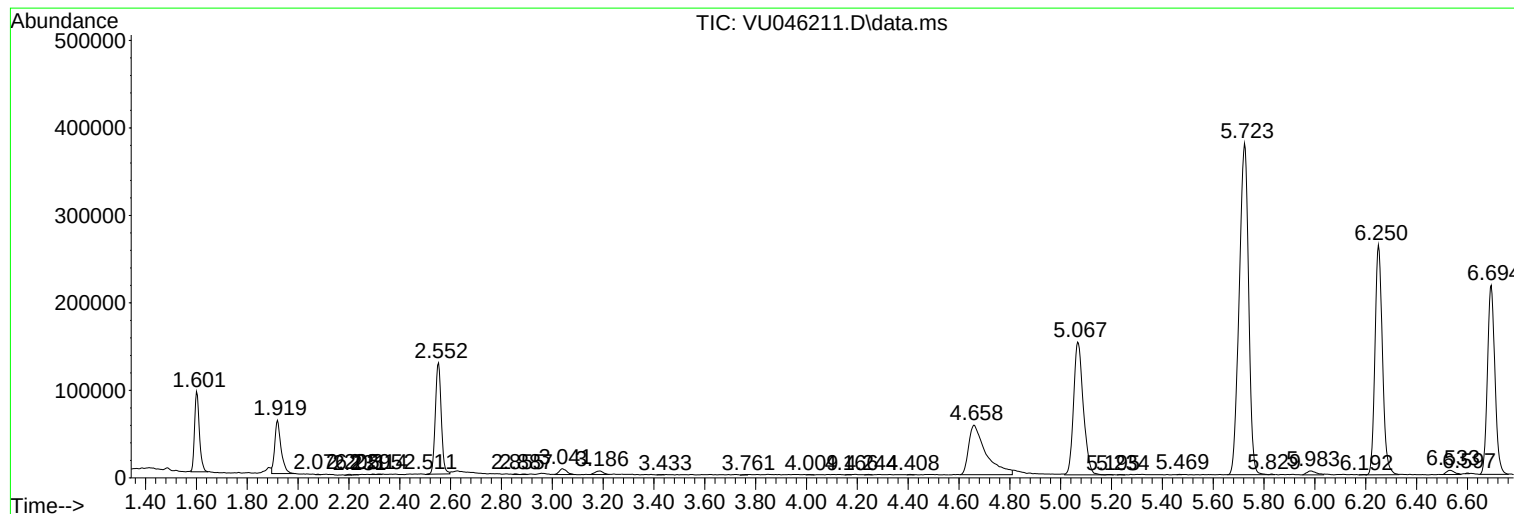
Sum of corrected areas: 8459230

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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 Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
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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