

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046331.D
 Acq On : 13 Dec 2021 21:12
 Operator : SY/MD
 Sample : M5023-01ME
 Misc : 6.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKX7ME

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: VU046331.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	101	rVB	64708	94104	15.95%	1.955%
2	1.916	172	179	206	rVB	34909	68467	11.60%	1.423%
3	2.060	221	224	228	rBV4	756	675	0.11%	0.014%
4	2.546	364	375	389	rBV	112631	182101	30.86%	3.784%
5	2.809	454	457	459	rBV2	533	324	0.05%	0.007%
6	2.864	470	474	479	rVB3	385	357	0.06%	0.007%
7	3.044	520	530	539	rBV5	1846	3538	0.60%	0.074%
8	3.105	545	549	552	rVB2	499	390	0.07%	0.008%
9	3.179	559	572	593	rBV	8438	22840	3.87%	0.475%
10	3.401	636	641	645	rVB2	283	321	0.05%	0.007%
11	3.591	697	700	703	rVB	491	360	0.06%	0.007%
12	3.742	743	747	750	rBV2	400	378	0.06%	0.008%
13	3.793	760	763	767	rVB	527	378	0.06%	0.008%
14	3.864	778	785	788	rBV	376	456	0.08%	0.009%
15	3.883	788	791	795	rVB	407	318	0.05%	0.007%
16	3.912	796	800	803	rBV2	385	316	0.05%	0.007%
17	4.041	832	840	844	rVB	347	452	0.08%	0.009%
18	4.108	856	861	867	rBV	513	575	0.10%	0.012%
19	4.472	971	974	978	rVB	428	335	0.06%	0.007%
20	4.504	978	984	989	rBV	486	728	0.12%	0.015%
21	4.661	1016	1033	1075	rBV2	265			

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 Title : VOC Analysis

37	7.484	1904	1911	1915	rVB	401	507	0.09%	0.011%
38	7.517	1915	1921	1924	rBV	308	310	0.05%	0.006%
39	7.568	1924	1937	1966	rVV	65642	132100	22.38%	2.745%
40	7.668	1966	1968	1972	rVB	608	372	0.06%	0.008%
41	7.697	1972	1977	1983	rBV	562	738	0.13%	0.015%
42	7.780	2000	2003	2007	rBV3	620	717	0.12%	0.015%
43	7.899	2026	2040	2057	rBV	246773	466108	78.98%	9.685%
44	8.185	2116	2129	2153	rBV	38524	88400	14.98%	1.837%
45	8.353	2178	2181	2189	rBV2	572	678	0.11%	0.014%
46	8.610	2256	2261	2262	rBV	449	367	0.06%	0.008%
47	8.684	2263	2284	2310	rVV	85874	270363	45.81%	5.618%
48	8.787	2313	2316	2320	rVB3	484	331	0.06%	0.007%
49	9.179	2434	2438	2442	rVB	496	476	0.08%	0.010%
50	9.211	2442	2448	2451	rBV	529	556	0.09%	0.012%
51	9.426	2496	2515	2537	rVV	241243	536209	90.86%	11.142%
52	9.526	2543	2546	2551	rBV2	399	467	0.08%	0.010%
53	9.738	2609	2612	2616	rBV2	532	356	0.06%	0.007%
54	9.951	2674	2678	2684	rVB	378	371	0.06%	0.008%
55	9.999	2690	2693	2701	rVB2	414	569	0.10%	0.012%
56	10.041	2701	2706	2709	rBV	389	380	0.06%	0.008%
57	10.150	2736	2740	2744	rBV	499	468	0.08%	0.010%
58	10.27								

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

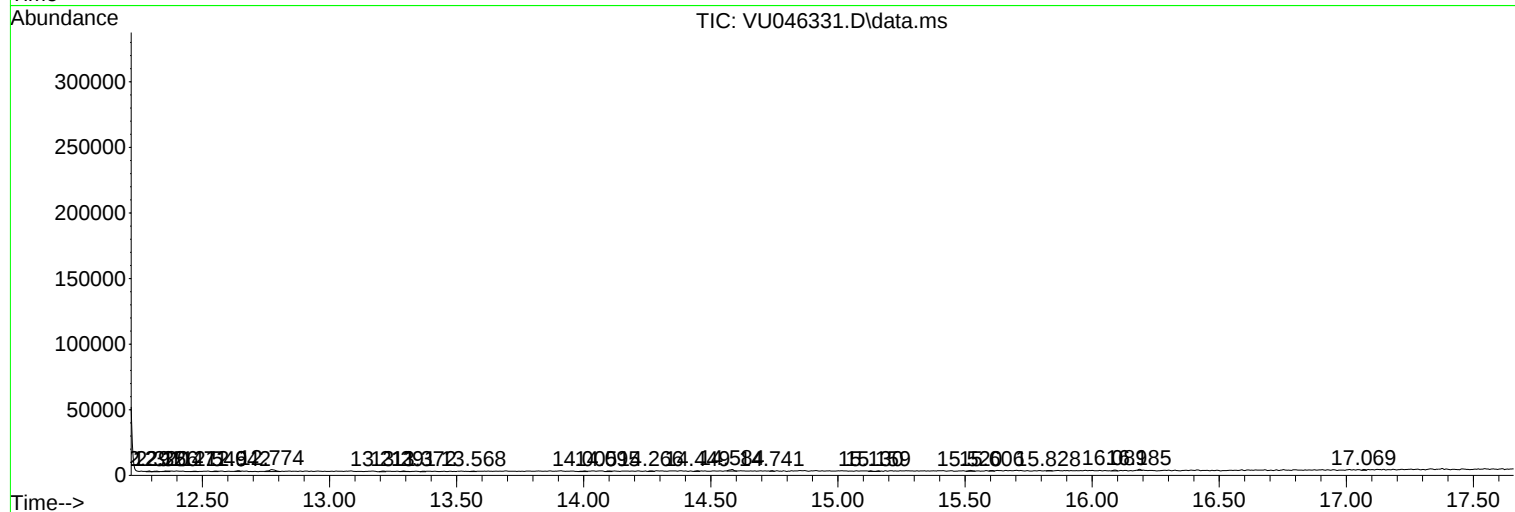
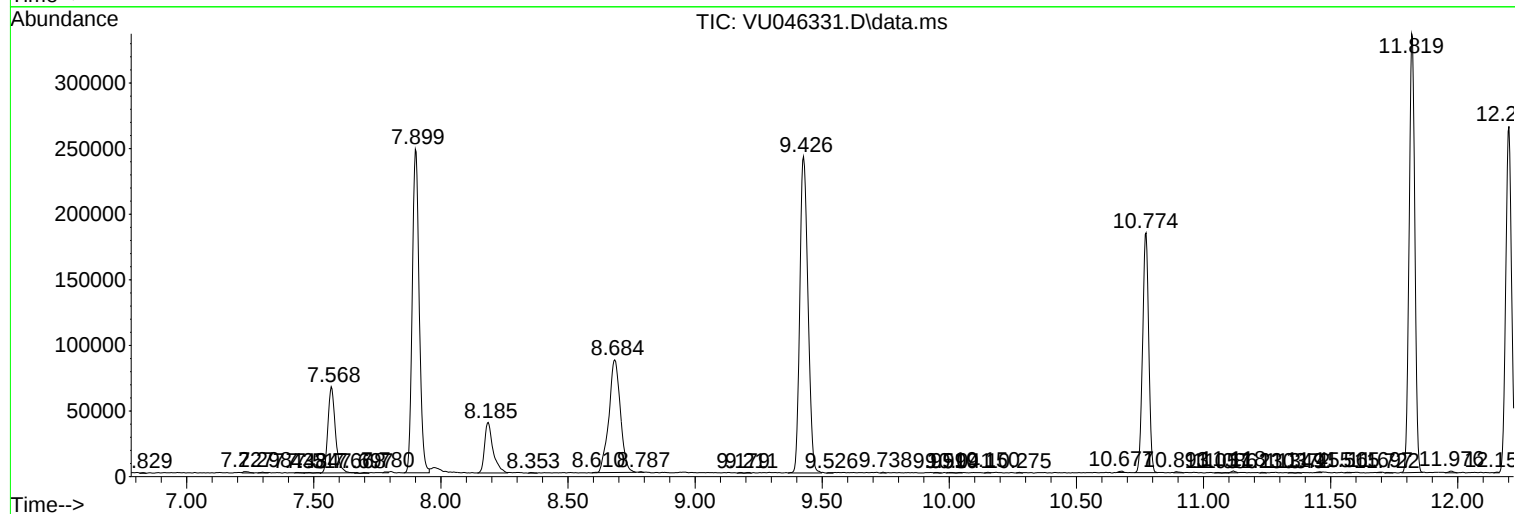
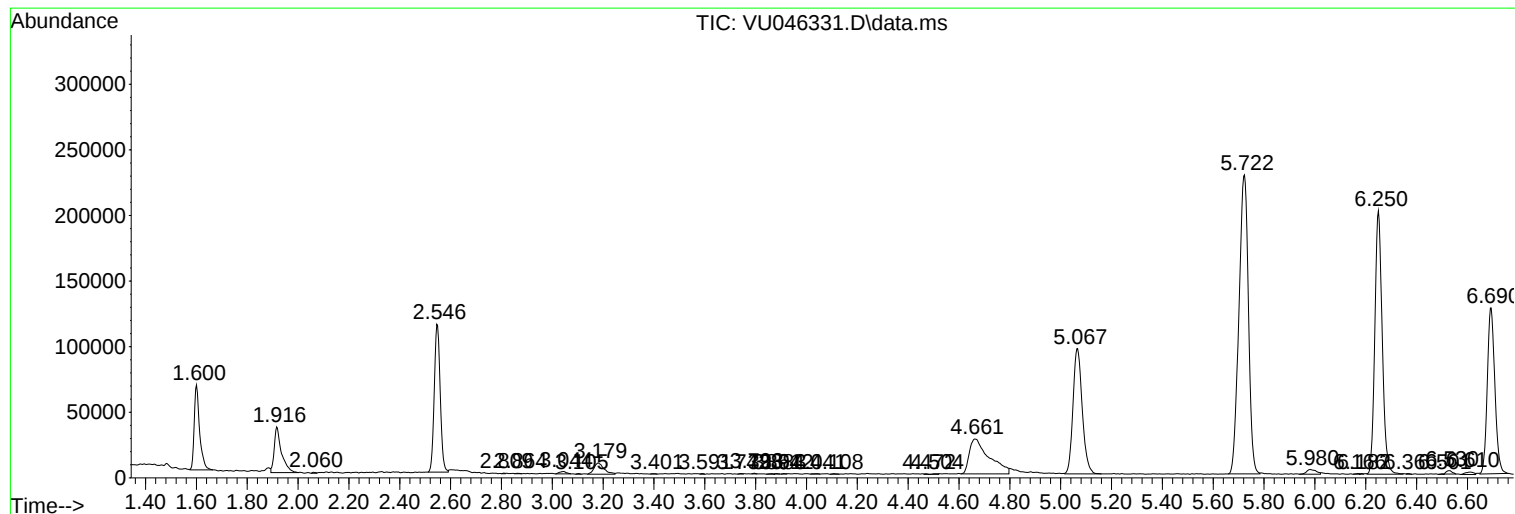
77	12.320	3409	3415	3418	rBV	415	468	0.08%	0.010%
78	12.356	3421	3426	3431	rBV	474	664	0.11%	0.014%
79	12.471	3456	3462	3466	rBV	299	313	0.05%	0.007%
80	12.549	3483	3486	3490	rBV	350	311	0.05%	0.006%
81	12.642	3510	3515	3518	rBV	588	513	0.09%	0.011%
82	12.774	3547	3556	3566	rVB3	1458	2567	0.43%	0.053%
83	13.211	3687	3692	3695	rBV2	493	516	0.09%	0.011%
84	13.291	3712	3717	3725	rBV2	460	523	0.09%	0.011%
85	13.372	3737	3742	3744	rBV	349	341	0.06%	0.007%
86	13.568	3798	3803	3806	rBV2	333	347	0.06%	0.007%
87	14.005	3931	3939	3942	rBV2	451	542	0.09%	0.011%
88	14.095	3964	3967	3972	rBV2	437	524	0.09%	0.011%
89	14.266	4016	4020	4024	rBV2	349	395	0.07%	0.008%
90	14.449	4072	4077	4079	rBV2	490	445	0.08%	0.009%
91	14.584	4113	4119	4125	rVB3	1219	1425	0.24%	0.030%
92	14.741	4165	4168	4171	rVB	521	311	0.05%	0.006%
93	15.130	4286	4289	4294	rVB2	556	373	0.06%	0.008%
94	15.159	4294	4298	4300	rBV2	452	331	0.06%	0.007%
95	15.520	4405	4410	4416	rBV3	653	796	0.13%	0.017%
96	15.606	4433							

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

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	#	RT	Resp	Conc
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