

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121421\
 Data File : VU046358.D
 Acq On : 14 Dec 2021 16:05
 Operator : SY/MD
 Sample : M5062-04ME
 Misc : 6.96g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

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: VU046358.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	74	81	88	rBV	32208	45160	8.37%	0.969%
2	1.919	172	180	189	rBV	17651	30212	5.60%	0.648%
3	2.549	366	376	391	rBV	82269	137828	25.54%	2.957%
4	2.967	503	506	515	rVV3	273	366	0.07%	0.008%
5	3.038	521	528	540	rVB4	1430	2924	0.54%	0.063%
6	3.179	560	572	583	rBV	3570	8304	1.54%	0.178%
7	3.314	611	614	617	rBV	187	192	0.04%	0.004%
8	3.388	631	637	639	rBV	157	209	0.04%	0.004%
9	3.636	711	714	717	rBB	161	131	0.02%	0.003%
10	3.665	718	723	726	rBV	173	235	0.04%	0.005%
11	3.829	771	774	778	rBB	152	151	0.03%	0.003%
12	3.864	778	785	793	rBB2	371	671	0.12%	0.014%
13	3.932	801	806	808	rBB	165	153	0.03%	0.003%
14	3.973	813	819	822	rBV	148	197	0.04%	0.004%
15	4.173	878	881	884	rBB	170	134	0.02%	0.003%
16	4.259	905	908	910	rBV	260	158	0.03%	0.003%
17	4.288	914	917	920	rVB	181	143	0.03%	0.003%
18	4.394	948	950	953	rBV	162	132	0.02%	0.003%
19	4.427	958	960	965	rBB	139	143	0.03%	0.003%
20	4.504	979	984	989	rBV	161	278	0.05%	0.006%
21	4.607	1011	1016	1017	rBV	274	182	0.03%	0.004%
22	4.658	1017	1032	1048	rBV	25878	92250	17.09%	1.979%
23	5.067	1142	1159	1190	rVB	92132	217056	40.22%	4.657%
24	5.195	1196	1199	1201	rBV	145	125	0.02%	0.003%
25	5.314	1222	1236	1251	rVB2	17542	38539	7.14%	0.827%
26	5.407	1263	1265	1269	rBV	129	138	0.03%	0.003%
27	5.452	1275	1279	1283	rBV	286	309	0.06%	0.007%
28	5.648	1336	1340	1343	rBV	147	143	0.03%	0.003%
29	5.722	1343	1363	1385	rVV2	213188	539726	100.00%	11.581%
30	5.980	1433	1443	1459	rBV6	3139	7492	1.39%	0.161%
31	6.169	1497	1502	1506	rBV2	304	416	0.08%	0.009%
32	6.195	1507	1510	1512	rVV2	329	267	0.05%	0.006%
33	6.250	1514	1527	1560	rVB	199761	400573	74.22%	8.595%
34	6.365	1560	1563	1565	rBV	267	168	0.03%	0.004%
35	6.536	1609	1616	1617	rBV4	2941	3092	0.57%	0.066%
36	6.600	1627	1636	1638	rBV2	1288	1640	0.30%	0.035%

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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

37	6.690	1651	1664	1687	rVB2	116165	239492	44.37%	5.139%
38	6.803	1697	1699	1704	rVB2	371	302	0.06%	0.006%
39	6.835	1705	1709	1711	rBB	167	135	0.03%	0.003%
40	7.002	1758	1761	1763	rBV	158	134	0.02%	0.003%
41	7.060	1777	1779	1782	rBV	135	123	0.02%	0.003%
42	7.214	1824	1827	1829	rBV2	254	148	0.03%	0.003%
43	7.227	1829	1831	1833	rVV3	294	151	0.03%	0.003%
44	7.266	1841	1843	1847	rBB	157	130	0.02%	0.003%
45	7.291	1847	1851	1852	rBV	260	190	0.04%	0.004%
46	7.343	1863	1867	1871	rBB	129	134	0.02%	0.003%
47	7.378	1875	1878	1882	rBB	146	154	0.03%	0.003%
48	7.500	1912	1916	1920	rBV	164	211	0.04%	0.005%
49	7.568	1925	1937	1960	rVV2	59086	116209	21.53%	2.494%
50	7.703	1976	1979	1983	rVB	156	137	0.03%	0.003%
51	7.793	1999	2007	2018	rBV2	900	2151	0.40%	0.046%
52	7.899	2026	2040	2057	rBV	219629	418890	77.61%	8.988%
53	8.099	2099	2102	2104	rBV	143	126	0.02%	0.003%
54	8.185	2117	2129	2155	rBV2	33470	77513	14.36%	1.663%
55	8.291	2160	2162	2165	rBV	140	124	0.02%	0.003%
56	8.404	2193	2197	2200	rBV	146	169	0.03%	0.004%
57	8.475	2208	2219	2230	rBV2	2277	4550	0.84%	0.098%
58	8.555	2232	2244	2259	rVB	131380	229948	42.60%	4.934%
59	8.687	2261	2285	2308	rBV2	82504	270884	50.19%	5.812%
60	8.799	2318	2320	2326	rVB3	258	181	0.03%	0.004%
61	8.947	2363	2366	2372	rVV2	274	301	0.06%	0.006%
62	9.205	2441	2446	2449	rBV	155	202	0.04%	0.004%
63	9.243	2454	2458	2461	rBB	158	130	0.02%	0.003%
64	9.266	2462	2465	2467	rBV	136	128	0.02%	0.003%
65	9.301	2474	2476	2481	rBV	231	186	0.03%	0.004%
66	9.426	2500	2515	2540	rBV	236268	534226	98.98%	11.463%
67	9.581	2559	2563	2566	rVB	191	165	0.03%	0.004%
68	9.693	2594	2598	2599	rVV2	206	163	0.03%	0.003%
69	9.706	2599	2602	2606	rVB2	309	278	0.05%	0.006%
70	9.918	2665	2668	2670	rBV	162	127	0.02%	0.003%
71	9.979	2684	2687	2692	rVB	180	214	0.04%	0.005%
72	10.041	2703	2706	2708	rBV	160	136	0.03%	0.003%
73	10.227	2762	2764	2769	rBB	168	165	0.03%	0.004%
74	10.356	2800	2804	2809	rBV	184	245	0.05%	0.005%
75	10.658	2894	2898	2900	rBV	304	228	0.04%	0.005%
76	10.674	2900	2903	2909	rVB2	750	749	0.14%	0.016%

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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

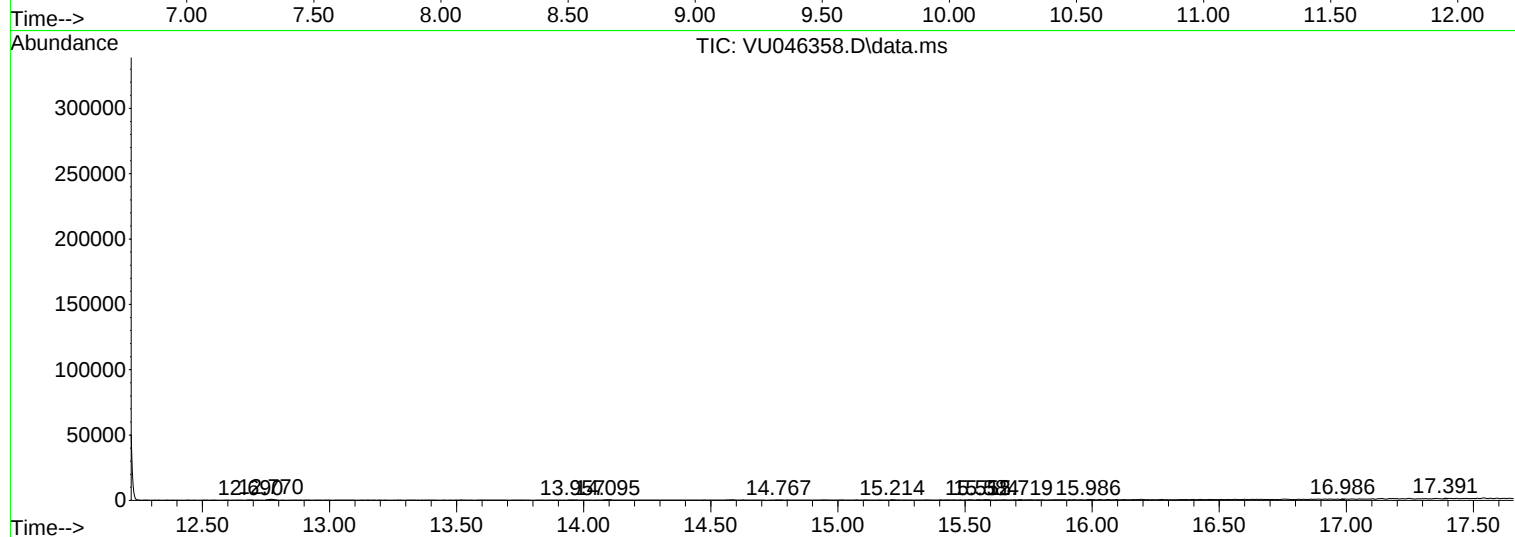
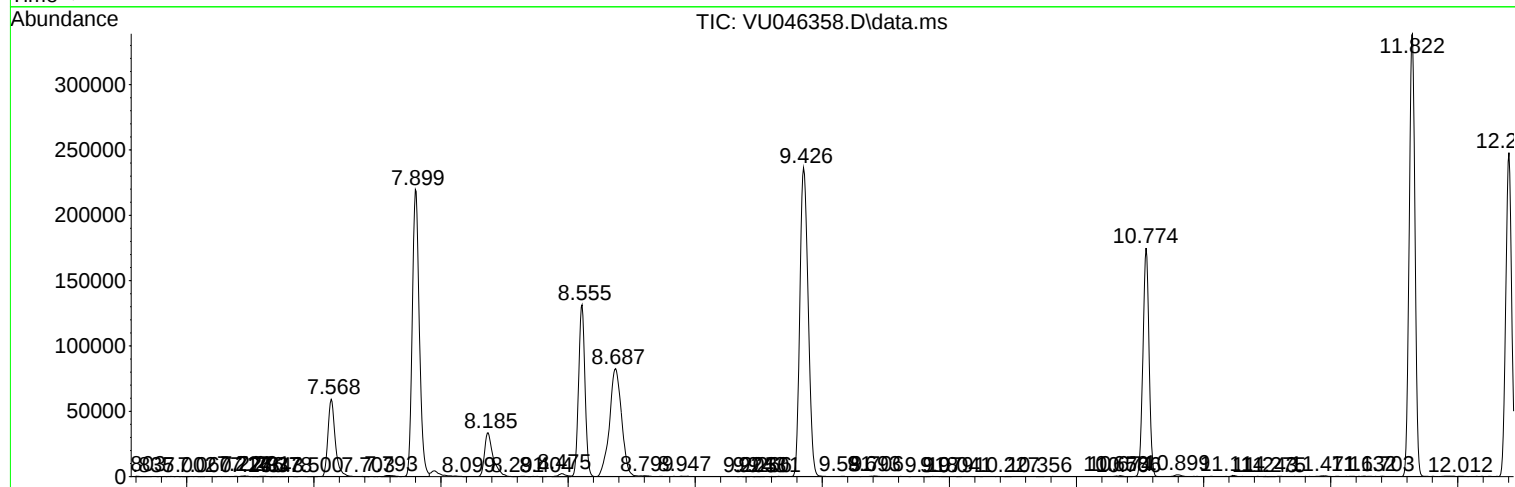
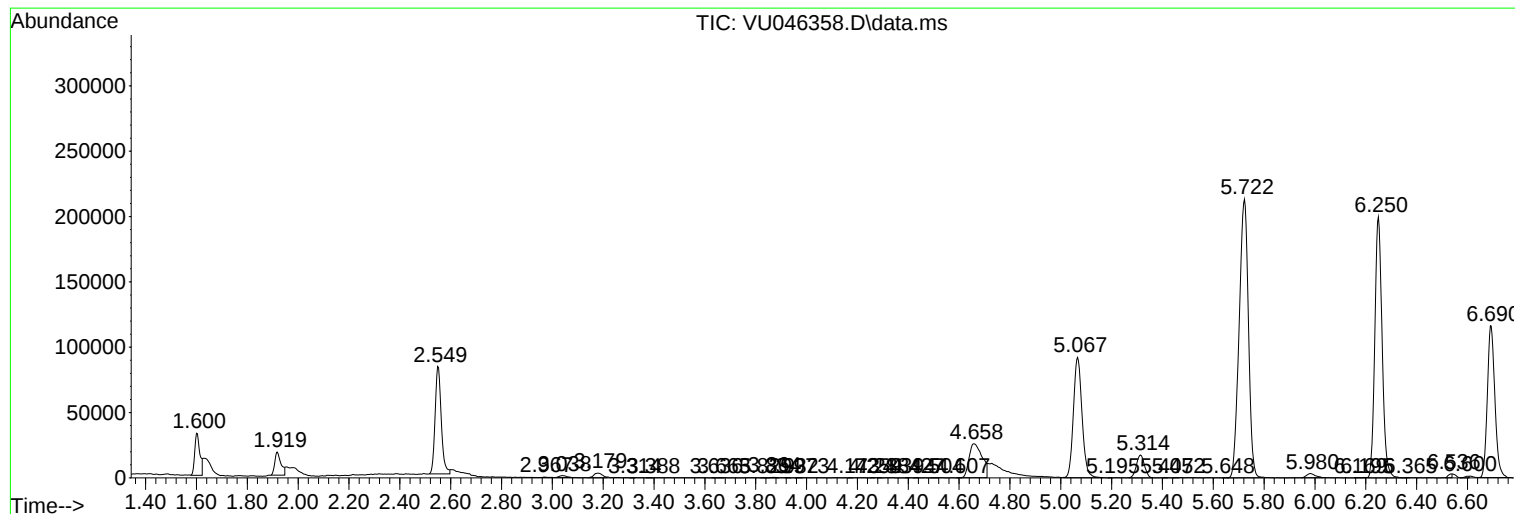
77	10.706	2909	2913	2917	rBV	166	216	0.04%	0.005%
78	10.774	2920	2934	2949	rVB	174872	293156	54.32%	6.290%
79	10.899	2964	2973	2984	rVB2	1292	2299	0.43%	0.049%
80	11.114	3035	3040	3047	rVB3	857	853	0.16%	0.018%
81	11.243	3078	3080	3083	rVB	199	125	0.02%	0.003%
82	11.275	3084	3090	3092	rBV	178	229	0.04%	0.005%
83	11.471	3146	3151	3152	rBV2	273	232	0.04%	0.005%
84	11.632	3197	3201	3204	rBV	235	225	0.04%	0.005%
85	11.703	3219	3223	3226	rVB	183	142	0.03%	0.003%
86	11.822	3247	3260	3276	rBV	338747	533576	98.86%	11.449%
87	12.012	3314	3319	3325	rBV	112	164	0.03%	0.004%
88	12.201	3366	3378	3391	rBV	247728	396023	73.37%	8.497%
89	12.690	3524	3530	3534	rBV	106	141	0.03%	0.003%
90	12.770	3548	3555	3562	rVV2	631	947	0.18%	0.020%
91	13.957	3917	3924	3930	rBV	175	261	0.05%	0.006%
92	14.095	3961	3967	3972	rVB2	294	377	0.07%	0.008%
93	14.767	4171	4176	4181	rBV	130	168	0.03%	0.004%
94	15.214	4312	4315	4320	rVB2	226	169	0.03%	0.004%
95	15.552	4417	4420	4424	rVB2	175	147	0.03%	0.003%
96	15.584	4425	4430	4435	rVB2	242	240	0.04%	0.005%
97	15.719	4468	4472	4474	rBV	317	214	0.04%	0.005%
98	15.986	4552	4555	4563	rVB	256	254	0.05%	0.005%
99	16.986	4863	4866	4868	rBV2	382	265	0.05%	0.006%
100	17.391	4989	4992	4994	rBV3	576	379	0.07%	0.008%

Sum of corrected areas: 4660468

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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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No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
