

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU052820\
 Data File : VU038343.D
 Acq On : 28 May 2020 13:46
 Operator : JC/MD
 Sample : L2753-03ME
 Misc : 10.28g/5.0mL/100 uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampled :
 GAXE4ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM052820WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.527	53	58	71	rBV2	8950	10581	0.36%	0.042%
2	1.607	75	83	101	rVB	333427	414973	14.10%	1.637%
3	1.874	160	166	172	rBV5	11367	17487	0.59%	0.069%
4	1.922	173	181	196	rVV	210188	300919	10.22%	1.187%
5	2.568	369	382	394	rBV	638499	1038072	35.27%	4.095%
6	2.803	449	455	464	rVB2	3438	4730	0.16%	0.019%
7	2.986	504	512	519	rVV3	2769	4968	0.17%	0.020%
8	3.063	529	536	549	rVB5	2234	4813	0.16%	0.019%
9	3.208	568	581	598	rBV	20429	49553	1.68%	0.196%
10	3.462	658	660	662	rBV2	664	370	0.01%	0.001%
11	3.520	675	678	682	rVB2	491	342	0.01%	0.001%
12	3.552	682	688	690	rBV	720	646	0.02%	0.003%
13	3.661	717	722	725	rVB2	373	322	0.01%	0.001%
14	3.893	789	794	796	rBV	396	308	0.01%	0.001%
15	4.269	904	911	916	rBV2	409	438	0.01%	0.002%
16	4.359	935	939	942	rVB	457	310	0.01%	0.001%
17	4.430	958	961	966	rVB2	390	287	0.01%	0.001%
18	4.488	971	979	981	rBV2	579	680	0.02%	0.003%
19	4.684	1023	1040	1081	rVV	207674	813590	27.64%	3.210%
20	4.851	1084	1092	1133	rVB3	57836	171592	5.83%	0.677%
21	5.099	1151	1169	1193	rBV	476877	1098468	37.32%	4.334%
22	5.266	1219	1221	1223	rBV3	574	312	0.01%	0.001%
23	5.317	1235	1237	1243	rVV3	857	837	0.03%	0.003%
24	5.407	1255	1265	1274	rBV5	1964	3461	0.12%	0.014%
25	5.526	1297	1302	1306	rBV3	372	314	0.01%	0.001%
26	5.613	1324	1329	1331	rBV2	345	300	0.01%	0.001%
27	5.626	1331	1333	1339	rBV3	517	403	0.01%	0.002%
28	5.755	1351	1373	1402	rBV2	1153616	2943320	100.00%	11.612%
29	5.967	1434	1439	1442	rBV2	581	611	0.02%	0.002%
30	6.005	1449	1451	1452	rBV	969	471	0.02%	0.002%
31	6.073	1463	1472	1474	rBV4	1025	1355	0.05%	0.005%
32	6.086	1474	1476	1481	rVB3	747	660	0.02%	0.003%
33	6.144	1490	1494	1498	rVV3	815	668	0.02%	0.003%
34	6.279	1517	1536	1568	rBV	1003109	2032809	69.07%	8.020%

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Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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 Stop Thrs : 0

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM052820WMA.M
 Title : VOC Analysis

35	6.510	1605	1608	1613	rVB3	368	317	0.01%	0.001%
36	6.568	1613	1626	1641	rBV5	16275	40563	1.38%	0.160%
37	6.722	1658	1674	1698	rBV	626108	1284282	43.63%	5.067%
38	6.832	1706	1708	1716	rVB6	1716	1806	0.06%	0.007%
39	6.922	1732	1736	1738	rVV	512	393	0.01%	0.002%
40	6.951	1742	1745	1750	rVV3	516	454	0.02%	0.002%
41	6.976	1750	1753	1756	rVB2	449	300	0.01%	0.001%
42	7.185	1812	1818	1820	rBV3	682	554	0.02%	0.002%
43	7.211	1820	1826	1827	rBV3	1318	1169	0.04%	0.005%
44	7.298	1851	1853	1860	rVB4	793	547	0.02%	0.002%
45	7.365	1870	1874	1878	rVB2	403	380	0.01%	0.001%
46	7.391	1878	1882	1884	rBV2	529	396	0.01%	0.002%
47	7.504	1915	1917	1921	rBV2	408	296	0.01%	0.001%
48	7.594	1928	1945	1970	rBV	348277	680219	23.11%	2.684%
49	7.703	1976	1979	1981	rBV2	757	531	0.02%	0.002%
50	7.819	2004	2015	2023	rBV7	6410	13633	0.46%	0.054%
51	7.925	2032	2048	2086	rBV	1263982	2417163	82.12%	9.536%
52	8.205	2122	2135	2159	rBV	226999	464454	15.78%	1.832%
53	8.346	2174	2179	2183	rBV3	482	531	0.02%	0.002%
54	8.375	2183	2188	2192	rBV3	634	501	0.02%	0.002%
55	8.407	2195	2198	2202	rVB2	512	366	0.01%	0.001%
56	8.446	2205	2210	2212	rBV3	412	433	0.01%	0.002%
57	8.497	2219	2226	2229	rBV4	904	876	0.03%	0.003%
58	8.574	2234	2250	2267	rBV	745971	1305060	44.34%	5.149%
59	8.687	2268	2285	2319	rVB	718965	1709846	58.09%	6.746%
60	8.857	2335	2338	2339	rBV2	777	464	0.02%	0.002%
61	8.912	2352	2355	2358	rVB3	580	397	0.01%	0.002%
62	8.999	2379	2382	2385	rVB2	519	305	0.01%	0.001%
63	9.079	2402	2407	2410	rBV3	620	530	0.02%	0.002%
64	9.166	2428	2434	2437	rBV3	733	714	0.02%	0.003%
65	9.443	2504	2520	2553	rBV	1272372	2520987	85.65%	9.946%
66	9.590	2559	2566	2567	rBV5	1704	1694	0.06%	0.007%
67	9.652	2582	2585	2589	rBV2	442	380	0.01%	0.001%
68	9.716	2589	2605	2615	rVV4	3647	6730	0.23%	0.027%
69	9.828	2635	2640	2642	rBV	537	362	0.01%	0.001%
70	9.957	2677	2680	2682	rBV2	445	322	0.01%	0.001%
71	10.134	2724	2735	2746	rBV7	3000	5818	0.20%	0.023%

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 GAXE4ME

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\SOMULM052820WMA.M
 Title : VOC Analysis

72	10.211	2752	2759	2762	rBV	439	564	0.02%	0.002%
73	10.414	2819	2822	2827	rVB2	609	446	0.02%	0.002%
74	10.446	2827	2832	2835	rBV2	529	495	0.02%	0.002%
75	10.500	2844	2849	2852	rBV5	1056	1042	0.04%	0.004%
76	10.671	2895	2902	2904	rBV3	445	618	0.02%	0.002%
77	10.783	2923	2937	2955	rBV	847194	1372457	46.63%	5.415%
78	11.008	3003	3007	3008	rBV2	915	601	0.02%	0.002%
79	11.102	3028	3036	3038	rBV3	2382	2092	0.07%	0.008%
80	11.243	3077	3080	3082	rBV3	560	331	0.01%	0.001%
81	11.430	3135	3138	3142	rVB2	682	499	0.02%	0.002%
82	11.484	3149	3155	3164	rVB4	3744	5061	0.17%	0.020%
83	11.587	3183	3187	3190	rVB2	448	300	0.01%	0.001%
84	11.639	3197	3203	3206	rVB3	393	368	0.01%	0.001%
85	11.680	3212	3216	3218	rBV2	436	324	0.01%	0.001%
86	11.745	3230	3236	3238	rBV3	1366	1253	0.04%	0.005%
87	11.764	3238	3242	3249	rVV4	3075	3467	0.12%	0.014%
88	11.832	3249	3263	3281	rVV	1531003	2416614	82.11%	9.534%
89	11.915	3285	3289	3293	rBV4	864	796	0.03%	0.003%
90	12.211	3368	3381	3403	rBV	1335097	2107952	71.62%	8.316%
91	12.340	3416	3421	3422	rBV	3749	2254	0.08%	0.009%
92	12.616	3504	3507	3510	rBV2	468	378	0.01%	0.001%
93	13.249	3695	3704	3712	rVB6	3723	5389	0.18%	0.021%
94	13.397	3747	3750	3753	rBV3	673	549	0.02%	0.002%
95	13.838	3884	3887	3888	rBV2	845	494	0.02%	0.002%
96	13.873	3892	3898	3907	rVB5	6971	10528	0.36%	0.042%
97	14.121	3967	3975	3985	rVB	11374	17653	0.60%	0.070%
98	14.211	4000	4003	4005	rBV2	637	447	0.02%	0.002%
99	14.272	4019	4022	4028	rVB	937	873	0.03%	0.003%
100	14.368	4044	4052	4060	rBV5	7386	10165	0.35%	0.040%

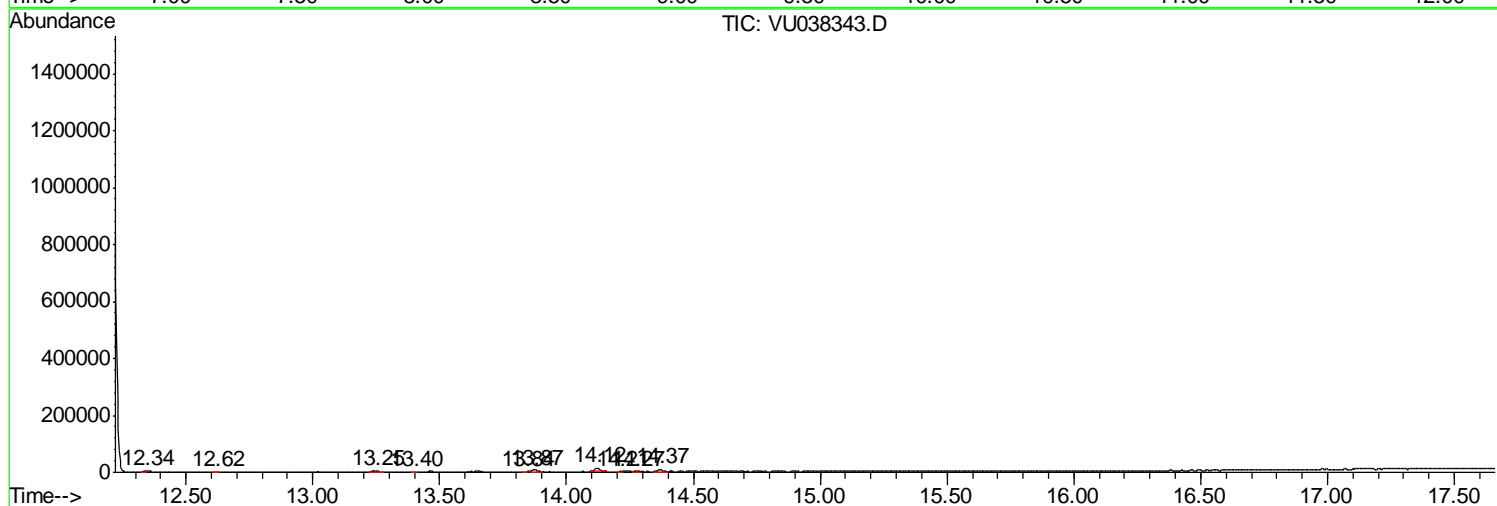
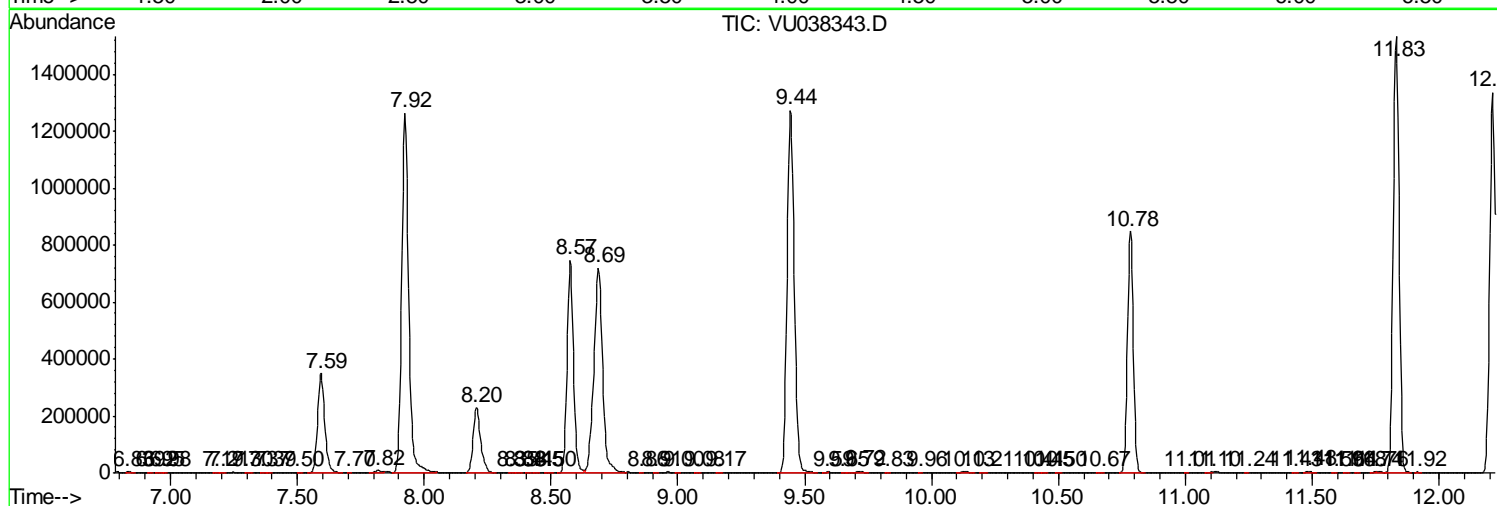
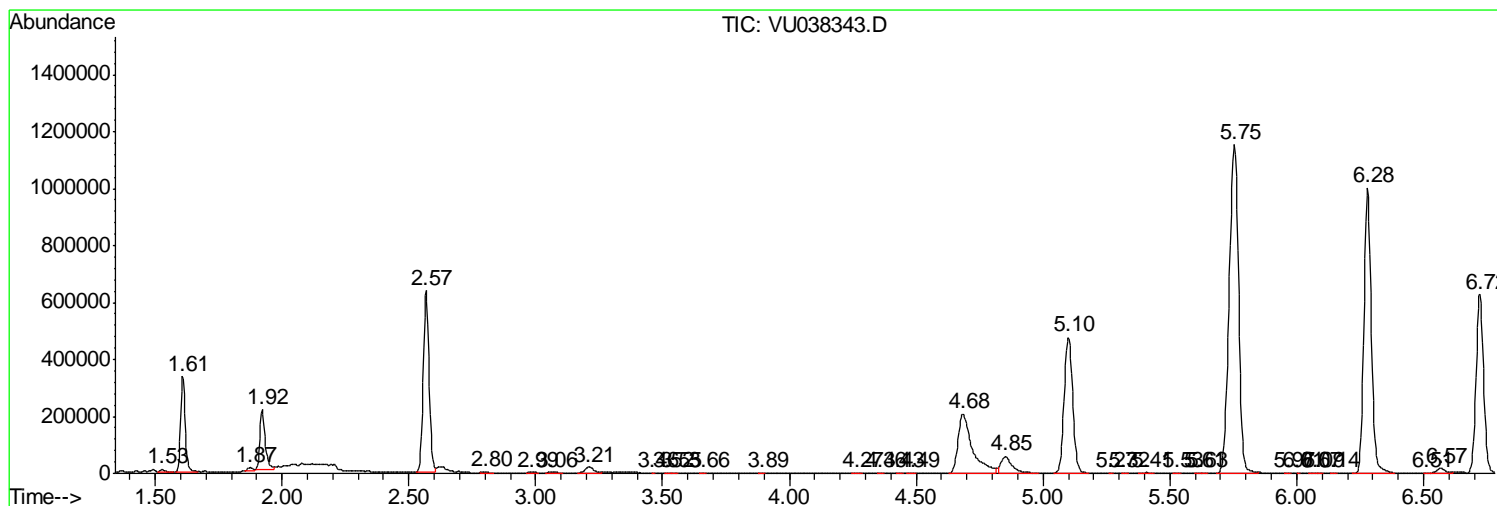
Sum of corrected areas: 25346753

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Instrument :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM052820WMA.M
 Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P



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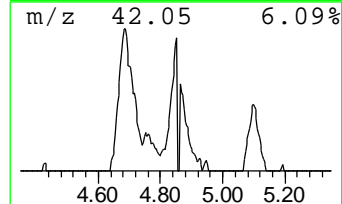
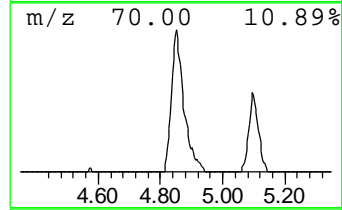
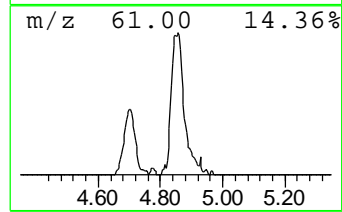
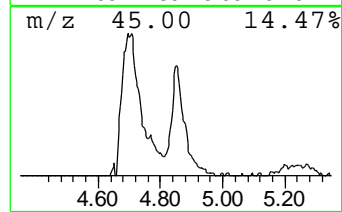
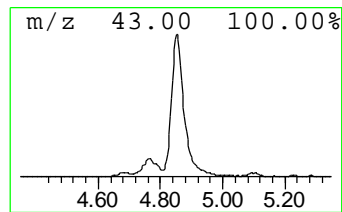
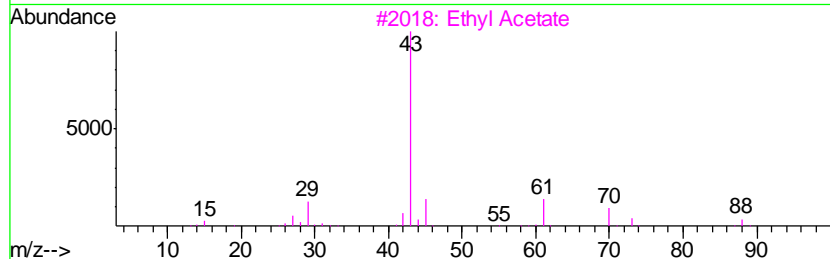
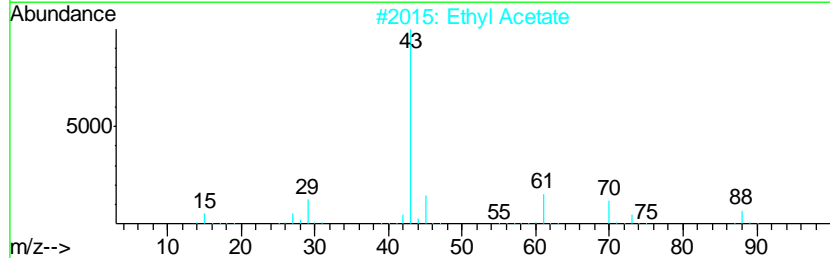
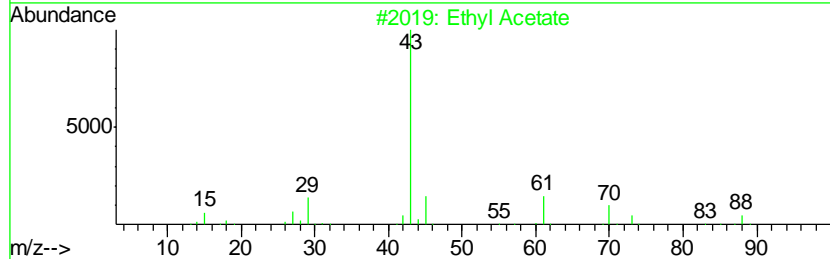
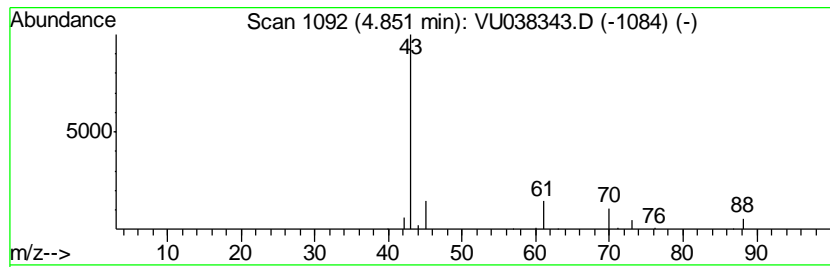
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM052820WMA.M
 Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 1 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	4.22 ug/L	171592	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	86
2		Ethyl Acetate	88	C4H8O2	000141-78-6	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	72
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.85	4.2	ug/L	171592	1	6.28	2032810	50.0