

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102821\
 Data File : VU045439.D
 Acq On : 28 Oct 2021 14:59
 Operator : SY/MD
 Sample : VU1028MBL07
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK035

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\SFAMULM102821WMA.M
 Title : VOC Analysis

Signal : TIC: VU045439.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	73	81	97	rVB	171171	186558	14.20%	1.876%
2	1.916	170	179	196	rVB	137898	179998	13.70%	1.810%
3	2.572	370	383	401	rBV	264108	437289	33.28%	4.398%
4	2.797	445	453	461	rBV2	930	1395	0.11%	0.014%
5	2.961	497	504	511	rBV3	420	676	0.05%	0.007%
6	3.047	526	531	539	rVB2	1165	1707	0.13%	0.017%
7	3.411	640	644	648	rBV2	219	204	0.02%	0.002%
8	3.485	662	667	671	rBV2	171	157	0.01%	0.002%
9	4.202	885	890	895	rBV2	144	176	0.01%	0.002%
10	4.408	951	954	958	rVB2	212	165	0.01%	0.002%
11	4.446	962	966	972	rVB2	194	214	0.02%	0.002%
12	4.494	976	981	983	rBV2	180	169	0.01%	0.002%
13	4.626	1005	1022	1056	rBV	148628	353760	26.92%	3.558%
14	4.922	1111	1114	1117	rVB2	196	152	0.01%	0.002%
15	4.948	1117	1122	1126	rBV3	344	342	0.03%	0.003%
16	5.067	1142	1159	1182	rVV	233482	505167	38.45%	5.081%
17	5.147	1182	1184	1190	rVB2	325	306	0.02%	0.003%
18	5.176	1190	1193	1195	rBV2	179	126	0.01%	0.001%
19	5.221	1203	1207	1210	rVB2	334	229	0.02%	0.002%
20	5.240	1210	1213	1217	rVB2	189	144	0.01%	0.001%
21	5.298	1217	1231	1236	rBV4	483	908	0.07%	0.009%
22	5.420	1262	1269	1273	rVB2	144	190	0.01%	0.002%
23	5.488	1285	1290	1295	rBV2	154	211	0.02%	0.002%
24	5.652	1335	1341	1342	rBV	187	134	0.01%	0.001%
25	5.729	1342	1365	1386	rBV2	486786	1313913	100.00%	13.216%
26	5.938	1427	1430	1434	rVB3	311	225	0.02%	0.002%
27	5.980	1440	1443	1448	rVB2	149	132	0.01%	0.001%
28	6.034	1458	1460	1465	rVB2	254	199	0.02%	0.002%
29	6.124	1482	1488	1492	rBV2	817	1117	0.09%	0.011%
30	6.253	1513	1528	1546	rBV	381106	719284	54.74%	7.235%
31	6.533	1607	1615	1626	rVB5	2501	4722	0.36%	0.047%
32	6.629	1641	1645	1650	rBV2	231	168	0.01%	0.002%
33	6.694	1650	1665	1688	rBV	313003	604533	46.01%	6.081%
34	6.813	1695	1702	1708	rBV5	772	976	0.07%	0.010%
35	6.989	1752	1757	1761	rVB3	225	195	0.01%	0.002%
36	7.044	1765	1774	1783	rBV3	716	1246	0.09%	0.013%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102821WMA.M
 Title : VOC Analysis

37	7.134	1792	1802	1807	rBV2	152	316	0.02%	0.003%
38	7.182	1808	1817	1827	rVV2	2739	4463	0.34%	0.045%
39	7.301	1850	1854	1858	rBV2	162	125	0.01%	0.001%
40	7.459	1897	1903	1906	rBV2	127	126	0.01%	0.001%
41	7.568	1924	1937	1954	rBV	176477	305021	23.21%	3.068%
42	7.687	1966	1974	1983	rBV4	2037	3455	0.26%	0.035%
43	7.796	2001	2008	2013	rVB3	585	753	0.06%	0.008%
44	7.903	2026	2041	2056	rBV	586553	1013717	77.15%	10.196%
45	8.060	2088	2090	2092	rVB2	268	142	0.01%	0.001%
46	8.182	2116	2128	2147	rVV	123004	207569	15.80%	2.088%
47	8.362	2181	2184	2190	rVB2	206	181	0.01%	0.002%
48	8.533	2234	2237	2240	rVV2	149	126	0.01%	0.001%
49	8.632	2253	2268	2303	rBV	436962	751139	57.17%	7.555%
50	9.208	2445	2447	2450	rVV2	233	140	0.01%	0.001%
51	9.420	2499	2513	2543	rVV	540595	885658	67.41%	8.908%
52	9.571	2556	2560	2570	rVB4	641	820	0.06%	0.008%
53	9.693	2589	2598	2604	rBV3	1052	1592	0.12%	0.016%
54	9.748	2609	2615	2619	rBV2	208	307	0.02%	0.003%
55	9.864	2647	2651	2656	rBV	157	142	0.01%	0.001%
56	9.947	2673	2677	2680	rBV2	154	135	0.01%	0.001%
57	10.009	2692	2696	2699	rBV	155	133	0.01%	0.001%
58	10.092	2719	2722	2724	rBV	159	131	0.01%	0.001%
59	10.108	2724	2727	2728	rBV	497	262	0.02%	0.003%
60	10.340	2797	2799	2802	rVB2	200	128	0.01%	0.001%
61	10.356	2802	2804	2807	rBV2	177	137	0.01%	0.001%
62	10.478	2839	2842	2852	rVB2	249	396	0.03%	0.004%
63	10.674	2894	2903	2911	rVV3	3358	4814	0.37%	0.048%
64	10.758	2916	2929	2948	rVV	421273	677507	51.56%	6.815%
65	10.873	2959	2965	2968	rBV4	637	785	0.06%	0.008%
66	11.041	3011	3017	3020	rBV2	192	216	0.02%	0.002%
67	11.089	3026	3032	3036	rBV3	704	796	0.06%	0.008%
68	11.121	3039	3042	3048	rVB5	847	881	0.07%	0.009%
69	11.150	3048	3051	3057	rVB3	626	517	0.04%	0.005%
70	11.189	3060	3063	3065	rBV	191	143	0.01%	0.001%
71	11.423	3133	3136	3139	rVB	331	177	0.01%	0.002%
72	11.459	3139	3147	3160	rBV2	2350	4347	0.33%	0.044%
73	11.700	3212	3222	3228	rBV3	1326	1999	0.15%	0.020%
74	11.745	3232	3236	3244	rVB4	937	1144	0.09%	0.012%
75	11.812	3244	3257	3281	rBV	534619	843960	64.23%	8.489%
76	11.944	3293	3298	3301	rVV5	985	1220	0.09%	0.012%

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Title : VOC Analysis

77	11.973	3302	3307	3314	rVB4	2132	2911	0.22%	0.029%
78	12.037	3321	3327	3331	rBV	238	261	0.02%	0.003%
79	12.060	3331	3334	3337	rBV2	147	134	0.01%	0.001%
80	12.118	3348	3352	3356	rBV3	289	308	0.02%	0.003%
81	12.195	3360	3376	3392	rVV	565004	897909	68.34%	9.031%
82	12.330	3413	3418	3425	rBV5	651	691	0.05%	0.007%
83	12.410	3440	3443	3446	rBV2	251	133	0.01%	0.001%
84	12.639	3510	3514	3520	rVB3	448	492	0.04%	0.005%
85	12.680	3524	3527	3531	rBV	218	137	0.01%	0.001%
86	12.912	3596	3599	3602	rBV2	321	274	0.02%	0.003%
87	12.996	3622	3625	3627	rBV2	191	134	0.01%	0.001%
88	13.070	3645	3648	3652	rBV3	505	391	0.03%	0.004%
89	13.115	3660	3662	3665	rBV3	189	128	0.01%	0.001%
90	13.147	3669	3672	3681	rVB4	448	540	0.04%	0.005%
91	13.227	3691	3697	3705	rVB4	498	722	0.05%	0.007%
92	13.822	3876	3882	3884	rBV2	214	256	0.02%	0.003%
93	13.838	3884	3887	3889	rBV	618	442	0.03%	0.004%
94	14.086	3959	3964	3965	rBV2	843	610	0.05%	0.006%
95	14.288	4024	4027	4031	rBV	279	201	0.02%	0.002%
96	14.369	4050	4052	4056	rVB2	269	161	0.01%	0.002%
97	14.581	4109	4118	4128	rBV3	992	1586	0.12%	0.016%
98	14.761	4172	4174	4179	rBV2	218	185	0.01%	0.002%
99	14.973	4235	4240	4243	rBV3	287	361	0.03%	0.004%
100	15.114	4280	4284	4287	rBV	391	366	0.03%	0.004%

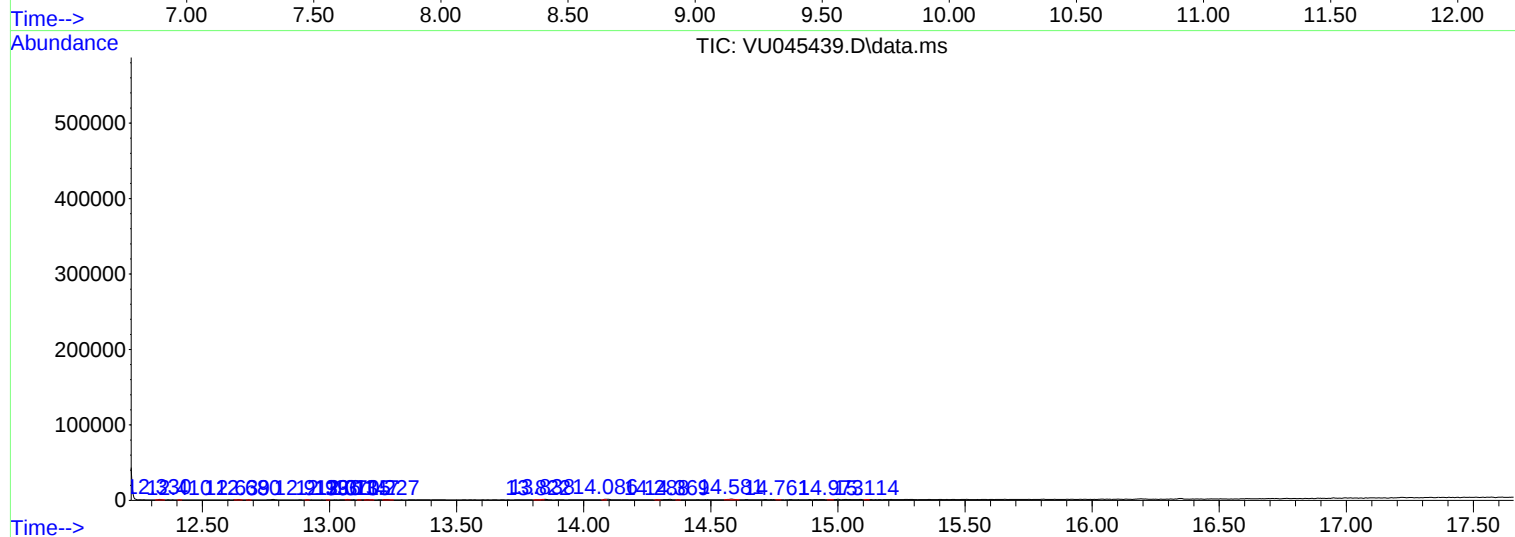
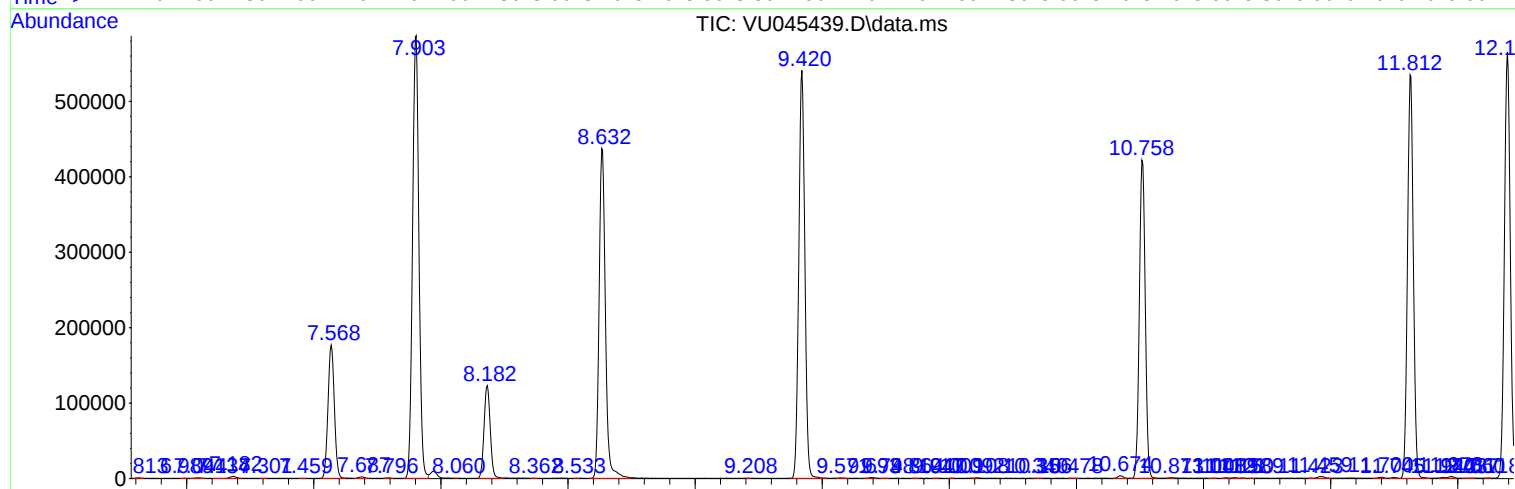
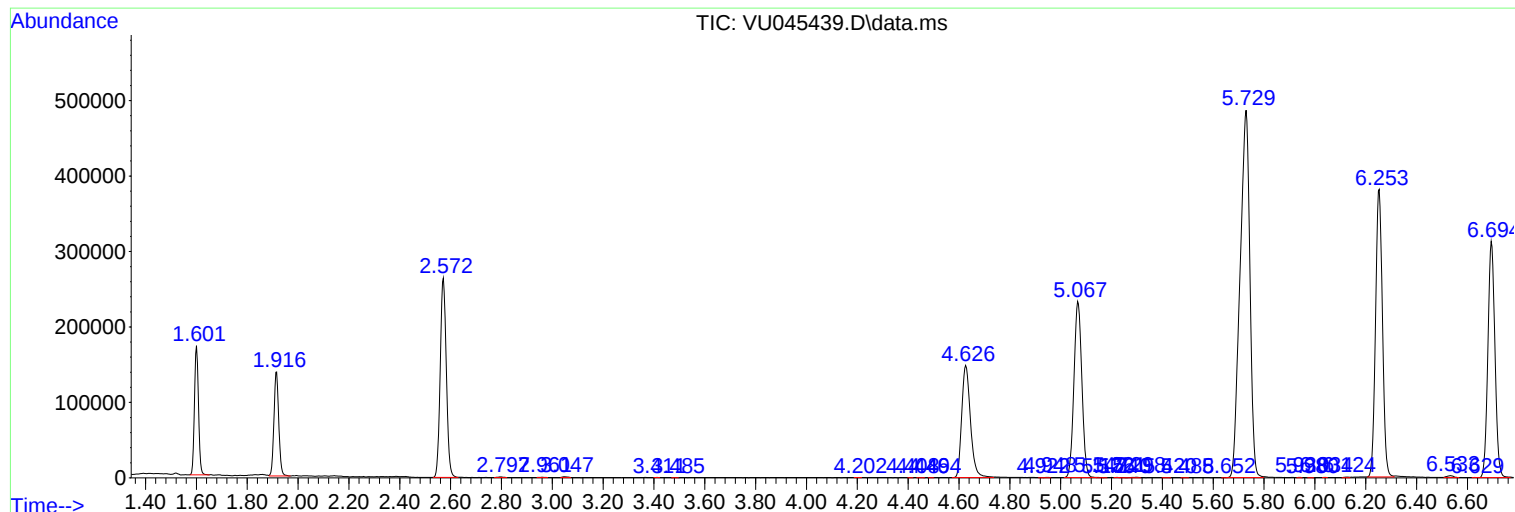
Sum of corrected areas: 9942040

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102821WMA.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\SFAMULM102821WMA.M
Quant Title : VOC Analysis

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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
