

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071822\
 Data File : VU049767.D
 Acq On : 18 Jul 2022 18:00
 Operator : SY/MD
 Sample : N3698-05MERE
 Misc : 4.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B70MERE

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\SFAMULM071122WMA.M

Title : VOC Analysis

Signal : TIC: VU049767.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	40	43	49	rVB5	1949	1756	0.17%	0.021%
2	1.594	71	79	85	rBV	45288	60159	5.72%	0.706%
3	1.867	122	164	172	rBV3	60467	203024	19.30%	2.383%
4	2.437	339	341	348	rVB4	1151	1051	0.10%	0.012%
5	2.520	354	367	380	rBV	144190	232579	22.11%	2.730%
6	2.604	390	393	397	rBV2	307	220	0.02%	0.003%
7	2.655	399	409	421	rVB4	1671	3368	0.32%	0.040%
8	2.703	421	424	431	rVB3	349	326	0.03%	0.004%
9	2.742	431	436	439	rBV2	539	558	0.05%	0.007%
10	2.877	475	478	481	rBV2	231	207	0.02%	0.002%
11	2.916	486	490	492	rBV2	433	412	0.04%	0.005%
12	2.951	496	501	505	rBV4	475	666	0.06%	0.008%
13	3.031	512	526	539	rVB6	3830	8648	0.82%	0.101%
14	3.173	555	570	589	rBV	26970	63349	6.02%	0.744%
15	3.330	616	619	620	rBV2	513	205	0.02%	0.002%
16	3.369	630	631	635	rVB2	522	234	0.02%	0.003%
17	3.658	718	721	722	rBV2	455	252	0.02%	0.003%
18	3.973	815	819	824	rVB2	283	291	0.03%	0.003%
19	4.002	824	828	831	rBV2	286	246	0.02%	0.003%
20	4.134	867	869	873	rBV2	259	204	0.02%	0.002%
21	4.269	907	911	916	rBV2	244	285	0.03%	0.003%
22	4.636	1009	1025	1076	rBV2	135313	449855	42.76%	5.280%
23	5.057	1140	1156	1180	rBV	193477	445181	42.32%	5.225%
24	5.276	1220	1224	1226	rBV3	497	385	0.04%	0.005%
25	5.375	1251	1255	1258	rBV2	489	433	0.04%	0.005%
26	5.446	1269	1277	1288	rVB5	1397	2870	0.27%	0.034%
27	5.575	1313	1317	1329	rVV3	664	812	0.08%	0.010%
28	5.713	1341	1360	1390	rBV2	404126	1051965	100.00%	12.347%
29	5.877	1406	1411	1412	rBV2	939	757	0.07%	0.009%
30	5.977	1431	1442	1462	rBV3	8411	20871	1.98%	0.245%
31	6.076	1470	1473	1482	rVB	336	367	0.03%	0.004%
32	6.243	1511	1525	1550	rVV	268660	525189	49.92%	6.164%
33	6.530	1604	1614	1625	rBV8	6038	11701	1.11%	0.137%
34	6.597	1627	1635	1649	rVV2	3788	7330	0.70%	0.086%
35	6.687	1649	1663	1691	rVB	260923	530202	50.40%	6.223%
36	6.790	1691	1695	1697	rBV3	959	791	0.08%	0.009%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

37	6.883	1718	1724	1726	rBV2	204	220	0.02%	0.003%
38	6.899	1726	1729	1736	rVB2	228	227	0.02%	0.003%
39	7.195	1810	1821	1823	rBV5	2985	4693	0.45%	0.055%
40	7.359	1868	1872	1876	rBV4	379	328	0.03%	0.004%
41	7.414	1882	1889	1892	rBV2	273	280	0.03%	0.003%
42	7.565	1920	1936	1954	rBV	125103	236741	22.50%	2.779%
43	7.690	1966	1975	1988	rBV6	1743	3146	0.30%	0.037%
44	7.790	1996	2006	2009	rBV3	642	936	0.09%	0.011%
45	7.832	2014	2019	2025	rVB2	453	468	0.04%	0.005%
46	7.896	2025	2039	2056	rBV	398983	705738	67.09%	8.283%
47	7.993	2060	2069	2082	rVB3	5390	10889	1.04%	0.128%
48	8.073	2089	2094	2101	rVB3	382	313	0.03%	0.004%
49	8.182	2113	2128	2147	rBV	85930	163324	15.53%	1.917%
50	8.346	2171	2179	2181	rBV4	413	539	0.05%	0.006%
51	8.652	2258	2274	2310	rBV2	381265	935027	88.88%	10.974%
52	8.944	2361	2365	2368	rBV3	347	331	0.03%	0.004%
53	9.185	2435	2440	2444	rVB2	196	208	0.02%	0.002%
54	9.224	2444	2452	2455	rVB2	329	379	0.04%	0.004%
55	9.420	2499	2513	2530	rBV	363879	657705	62.52%	7.719%
56	9.542	2547	2551	2556	rBV2	194	215	0.02%	0.003%
57	9.571	2556	2560	2562	rVV2	358	325	0.03%	0.004%
58	9.600	2566	2569	2575	rVV2	250	279	0.03%	0.003%
59	9.693	2593	2598	2601	rBV3	462	379	0.04%	0.004%
60	9.748	2610	2615	2619	rBV2	251	343	0.03%	0.004%
61	9.883	2648	2657	2661	rBV2	229	339	0.03%	0.004%
62	9.925	2667	2670	2677	rBV2	365	389	0.04%	0.005%
63	10.105	2722	2726	2730	rBV2	394	397	0.04%	0.005%
64	10.128	2730	2733	2740	rVB3	426	333	0.03%	0.004%
65	10.208	2754	2758	2762	rBV	284	229	0.02%	0.003%
66	10.246	2766	2770	2776	rVB2	207	224	0.02%	0.003%
67	10.761	2917	2930	2949	rBV	459601	756518	71.91%	8.879%
68	10.851	2956	2958	2965	rVB2	400	313	0.03%	0.004%
69	10.992	2999	3002	3008	rBV	200	197	0.02%	0.002%
70	11.092	3029	3033	3036	rVB4	325	233	0.02%	0.003%
71	11.115	3036	3040	3047	rBV3	718	789	0.08%	0.009%
72	11.314	3099	3102	3108	rBV	343	247	0.02%	0.003%
73	11.359	3113	3116	3121	rBV2	238	216	0.02%	0.003%
74	11.472	3146	3151	3153	rBV3	467	398	0.04%	0.005%
75	11.607	3189	3193	3194	rBV	348	241	0.02%	0.003%
76	11.706	3220	3224	3227	rBV2	274	203	0.02%	0.002%

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 Title : VOC Analysis

77	11.748	3234	3237	3240	rBV2	545	487	0.05%	0.006%
78	11.816	3246	3258	3275	rBV	383103	619397	58.88%	7.270%
79	11.928	3291	3293	3296	rVB2	602	267	0.03%	0.003%
80	12.195	3363	3376	3400	rBV	479965	774556	73.63%	9.091%
81	12.340	3417	3421	3422	rBV2	324	197	0.02%	0.002%
82	12.828	3570	3573	3577	rBV2	254	237	0.02%	0.003%
83	13.224	3692	3696	3699	rBV3	389	346	0.03%	0.004%
84	13.397	3747	3750	3753	rBV2	243	211	0.02%	0.002%
85	13.491	3777	3779	3785	rBV	237	195	0.02%	0.002%
86	13.690	3838	3841	3843	rBV2	351	197	0.02%	0.002%
87	13.796	3869	3874	3880	rBV3	416	494	0.05%	0.006%
88	13.854	3882	3892	3900	rBV4	1006	1628	0.15%	0.019%
89	14.063	3953	3957	3959	rBV2	273	216	0.02%	0.003%
90	14.092	3959	3966	3970	rBV3	2446	2899	0.28%	0.034%
91	14.169	3985	3990	3993	rBV2	334	360	0.03%	0.004%
92	14.214	4002	4004	4010	rBV	278	206	0.02%	0.002%
93	14.336	4038	4042	4049	rVB4	1495	1409	0.13%	0.017%
94	14.487	4086	4089	4091	rBV2	412	240	0.02%	0.003%
95	14.578	4107	4117	4123	rBV2	2423	3699	0.35%	0.043%
96	15.002	4245	4249	4254	rBV3	474	448	0.04%	0.005%
97	15.253	4324	4327	4331	rBV3	488	388	0.04%	0.005%
98	16.018	4563	4565	4570	rBV2	524	340	0.03%	0.004%
99	16.410	4685	4687	4689	rVB3	728	278	0.03%	0.003%
100	16.423	4689	4691	4694	rBV3	791	472	0.04%	0.006%

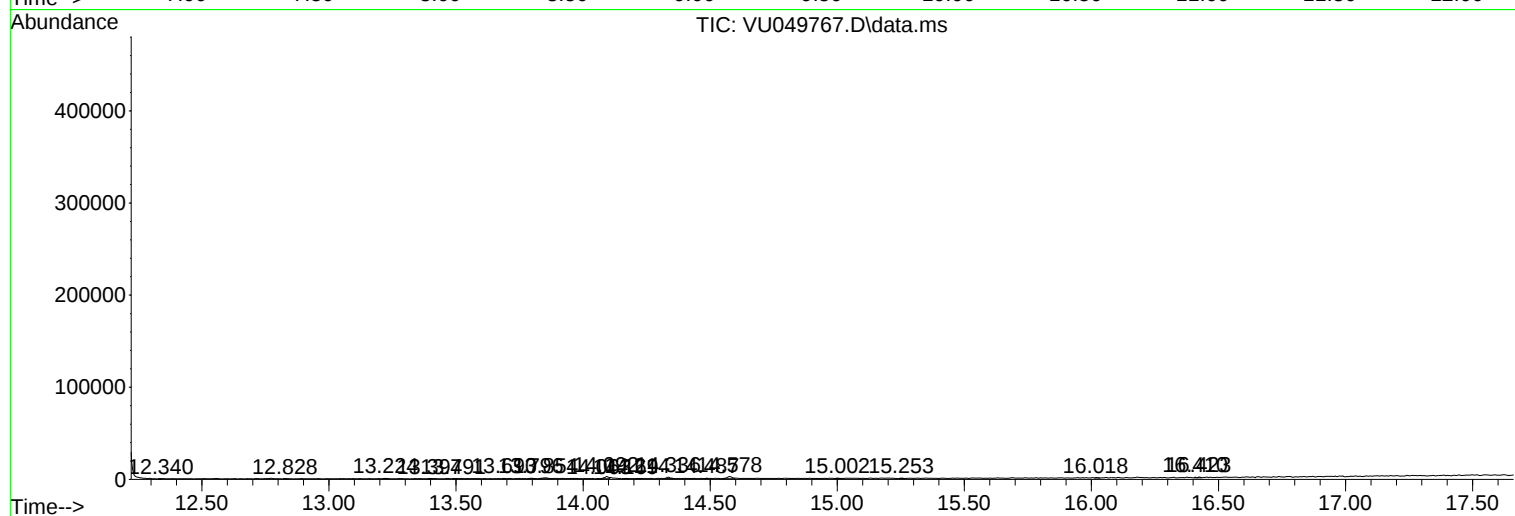
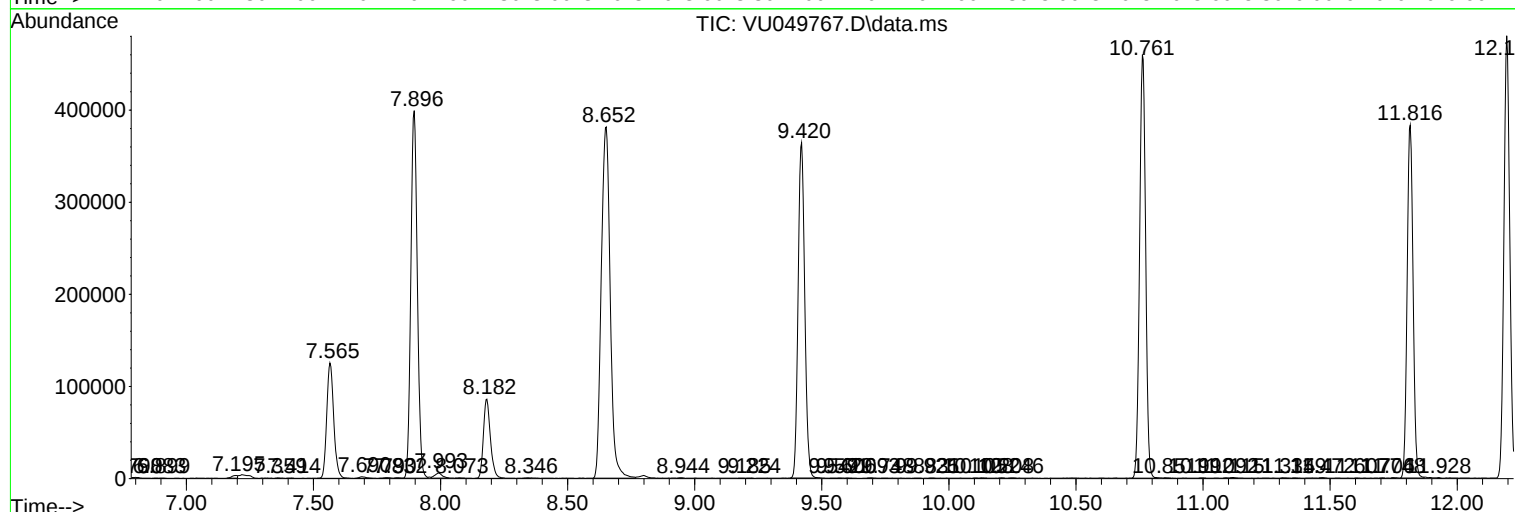
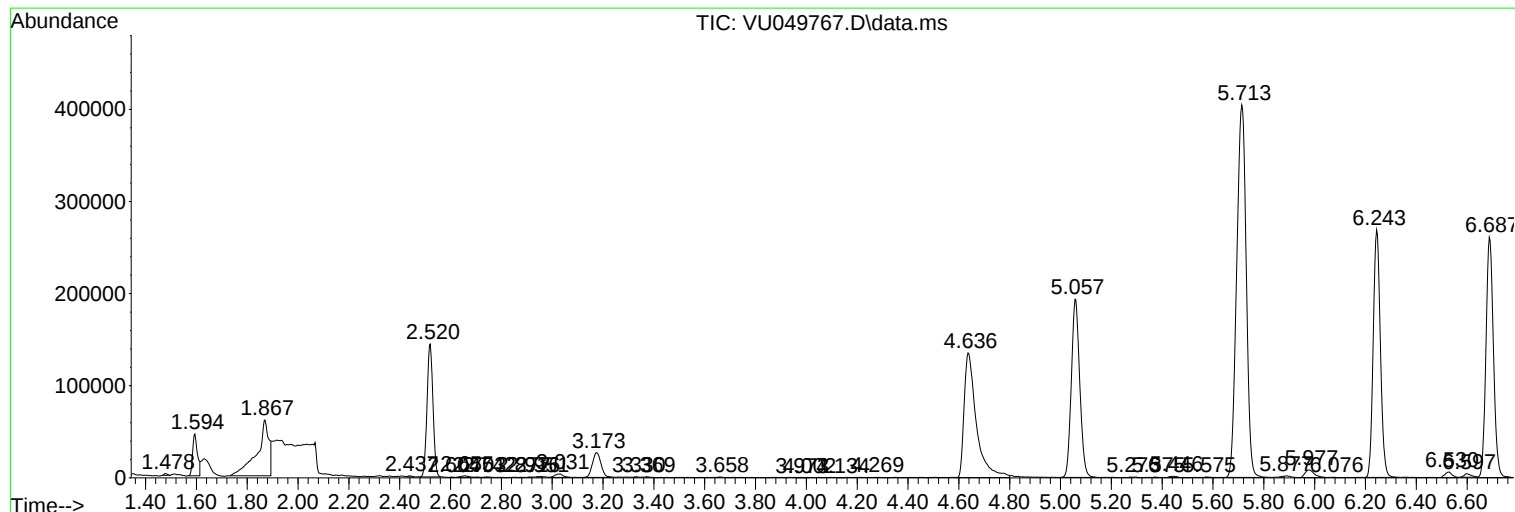
Sum of corrected areas: 8520215

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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\SFAMULM071122WMA.M
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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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