

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049799.D
 Acq On : 20 Jul 2022 12:11
 Operator : SY/MD
 Sample : N3698-11ME
 Misc : 3.79g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B76ME

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: VU049799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	40	44	49	rBV3	1997	1863	0.24%	0.031%
2	1.594	71	79	86	rBV	61852	82262	10.74%	1.349%
3	1.880	164	168	179	rBV	32422	33928	4.43%	0.557%
4	2.244	277	281	286	rVB4	1030	892	0.12%	0.015%
5	2.533	359	371	386	rBV	151848	244561	31.92%	4.012%
6	2.646	397	406	409	rBV3	1816	2571	0.34%	0.042%
7	2.755	434	440	449	rVB3	811	1168	0.15%	0.019%
8	2.954	492	502	505	rBV5	1505	2375	0.31%	0.039%
9	3.028	516	525	545	rVB2	7204	13468	1.76%	0.221%
10	3.176	556	571	595	rBV2	18943	44216	5.77%	0.725%
11	3.337	614	621	629	rVV6	1561	2670	0.35%	0.044%
12	3.440	649	653	658	rBV2	160	204	0.03%	0.003%
13	3.568	689	693	698	rVB2	356	343	0.04%	0.006%
14	3.601	698	703	708	rBV2	286	321	0.04%	0.005%
15	3.665	719	723	726	rBV3	495	551	0.07%	0.009%
16	3.961	812	815	819	rVB2	322	277	0.04%	0.005%
17	3.993	819	825	828	rBV2	325	358	0.05%	0.006%
18	4.099	854	858	863	rBV2	240	316	0.04%	0.005%
19	4.138	863	870	873	rVV2	280	351	0.05%	0.006%
20	4.160	873	877	883	rVV2	374	383	0.05%	0.006%
21	4.334	927	931	933	rBV2	251	199	0.03%	0.003%
22	4.414	952	956	962	rVB2	213	218	0.03%	0.004%
23	4.646	1012	1028	1058	rBV4	72355	250940	32.75%	4.116%
24	4.957	1121	1125	1128	rBV2	276	277	0.04%	0.005%
25	5.060	1141	1157	1183	rBV	136294	307230	40.10%	5.039%
26	5.202	1198	1201	1203	rBV	340	230	0.03%	0.004%
27	5.276	1221	1224	1226	rBV	317	252	0.03%	0.004%
28	5.716	1342	1361	1381	rBV2	299110	766233	100.00%	12.568%
29	5.977	1432	1442	1457	rBV5	6455	13818	1.80%	0.227%
30	6.247	1511	1526	1546	rBV	257524	495794	64.71%	8.132%
31	6.353	1557	1559	1562	rVB	412	235	0.03%	0.004%
32	6.379	1562	1567	1571	rBV2	207	249	0.03%	0.004%
33	6.526	1601	1613	1625	rBV9	4141	8149	1.06%	0.134%
34	6.597	1628	1635	1639	rBV3	2463	3493	0.46%	0.057%
35	6.690	1650	1664	1688	rVB	176566	354703	46.29%	5.818%
36	6.806	1696	1700	1702	rBV	476	326	0.04%	0.005%

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 Title : VOC Analysis

37	6.919	1731	1735	1742	rBV2	202	262	0.03%	0.004%
38	6.973	1745	1752	1756	rBV3	245	244	0.03%	0.004%
39	7.195	1812	1821	1822	rBV3	1949	2132	0.28%	0.035%
40	7.317	1856	1859	1862	rVB3	308	197	0.03%	0.003%
41	7.565	1924	1936	1964	rVV	86963	165618	21.61%	2.717%
42	7.694	1972	1976	1979	rBV3	549	548	0.07%	0.009%
43	7.790	2002	2006	2008	rBV3	500	440	0.06%	0.007%
44	7.896	2025	2039	2059	rBV	317602	580479	75.76%	9.522%
45	7.989	2063	2068	2083	rVB4	4647	9268	1.21%	0.152%
46	8.067	2088	2092	2093	rBV2	328	208	0.03%	0.003%
47	8.182	2115	2128	2153	rVB2	57886	110210	14.38%	1.808%
48	8.350	2175	2180	2184	rBV3	582	529	0.07%	0.009%
49	8.478	2217	2220	2224	rVB	258	196	0.03%	0.003%
50	8.546	2238	2241	2245	rBV2	359	210	0.03%	0.003%
51	8.568	2246	2248	2259	rVB2	189	215	0.03%	0.004%
52	8.655	2259	2275	2307	rBV2	189610	448932	58.59%	7.364%
53	8.800	2315	2320	2324	rBV4	1614	1676	0.22%	0.027%
54	8.899	2348	2351	2355	rVB	237	200	0.03%	0.003%
55	9.337	2483	2487	2492	rBV2	192	210	0.03%	0.003%
56	9.420	2500	2513	2530	rBV	347242	613850	80.11%	10.069%
57	9.571	2555	2560	2567	rBV3	652	667	0.09%	0.011%
58	9.703	2594	2601	2607	rVB3	521	701	0.09%	0.011%
59	9.919	2662	2668	2669	rBV2	208	219	0.03%	0.004%
60	10.105	2722	2726	2728	rBV2	309	236	0.03%	0.004%
61	10.340	2793	2799	2800	rBV	258	229	0.03%	0.004%
62	10.488	2840	2845	2848	rBV2	256	283	0.04%	0.005%
63	10.620	2883	2886	2892	rVB3	468	504	0.07%	0.008%
64	10.655	2892	2897	2900	rBV2	447	416	0.05%	0.007%
65	10.764	2917	2931	2949	rVV	251976	416620	54.37%	6.834%
66	11.028	3011	3013	3017	rVB2	345	252	0.03%	0.004%
67	11.066	3020	3025	3028	rVV2	203	221	0.03%	0.004%
68	11.086	3028	3031	3033	rVV	344	252	0.03%	0.004%
69	11.118	3033	3041	3050	rVB5	1368	1883	0.25%	0.031%
70	11.198	3062	3066	3070	rBV	341	253	0.03%	0.004%
71	11.359	3111	3116	3118	rBV	342	304	0.04%	0.005%
72	11.372	3118	3120	3123	rVV	525	233	0.03%	0.004%
73	11.816	3246	3258	3278	rBV	361527	574769	75.01%	9.428%
74	12.198	3363	3377	3399	rBV	316399	516019	67.34%	8.464%
75	12.275	3399	3401	3405	rVB2	382	263	0.03%	0.004%
76	12.298	3405	3408	3410	rBV2	357	198	0.03%	0.003%

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77	12.507	3468	3473	3475	rBV2	300	313	0.04%	0.005%
78	12.777	3551	3557	3558	rBV2	411	415	0.05%	0.007%
79	13.037	3634	3638	3640	rBV	248	196	0.03%	0.003%
80	13.099	3654	3657	3660	rBV	288	195	0.03%	0.003%
81	13.118	3660	3663	3666	rBV2	294	232	0.03%	0.004%
82	13.227	3692	3697	3701	rBV2	502	597	0.08%	0.010%
83	13.295	3716	3718	3721	rBV	285	201	0.03%	0.003%
84	13.410	3750	3754	3759	rVB2	426	363	0.05%	0.006%
85	13.436	3759	3762	3765	rBV	295	240	0.03%	0.004%
86	13.459	3765	3769	3776	rVV3	247	234	0.03%	0.004%
87	13.565	3798	3802	3804	rBV2	414	334	0.04%	0.005%
88	13.658	3825	3831	3836	rBV2	343	545	0.07%	0.009%
89	13.793	3869	3873	3880	rVB	286	296	0.04%	0.005%
90	13.848	3885	3890	3892	rBV	689	609	0.08%	0.010%
91	13.954	3919	3923	3925	rBV2	325	258	0.03%	0.004%
92	14.099	3961	3968	3979	rVB3	2043	2592	0.34%	0.043%
93	14.336	4038	4042	4044	rBV2	1076	814	0.11%	0.013%
94	14.375	4052	4054	4059	rBV2	403	294	0.04%	0.005%
95	14.520	4095	4099	4100	rBV2	344	254	0.03%	0.004%
96	14.767	4173	4176	4179	rBV2	333	326	0.04%	0.005%
97	15.121	4283	4286	4287	rBV	331	233	0.03%	0.004%
98	15.745	4478	4480	4485	rVB3	678	474	0.06%	0.008%
99	15.909	4529	4531	4534	rVB	438	216	0.03%	0.004%
100	16.179	4613	4615	4621	rVB3	877	661	0.09%	0.011%

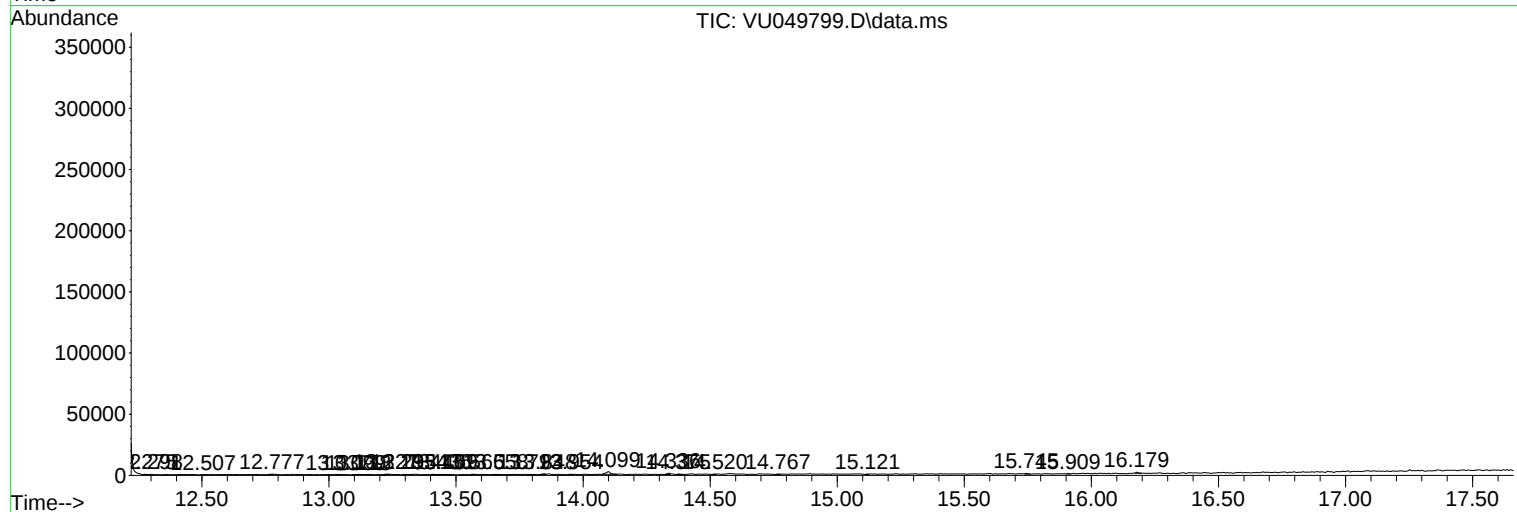
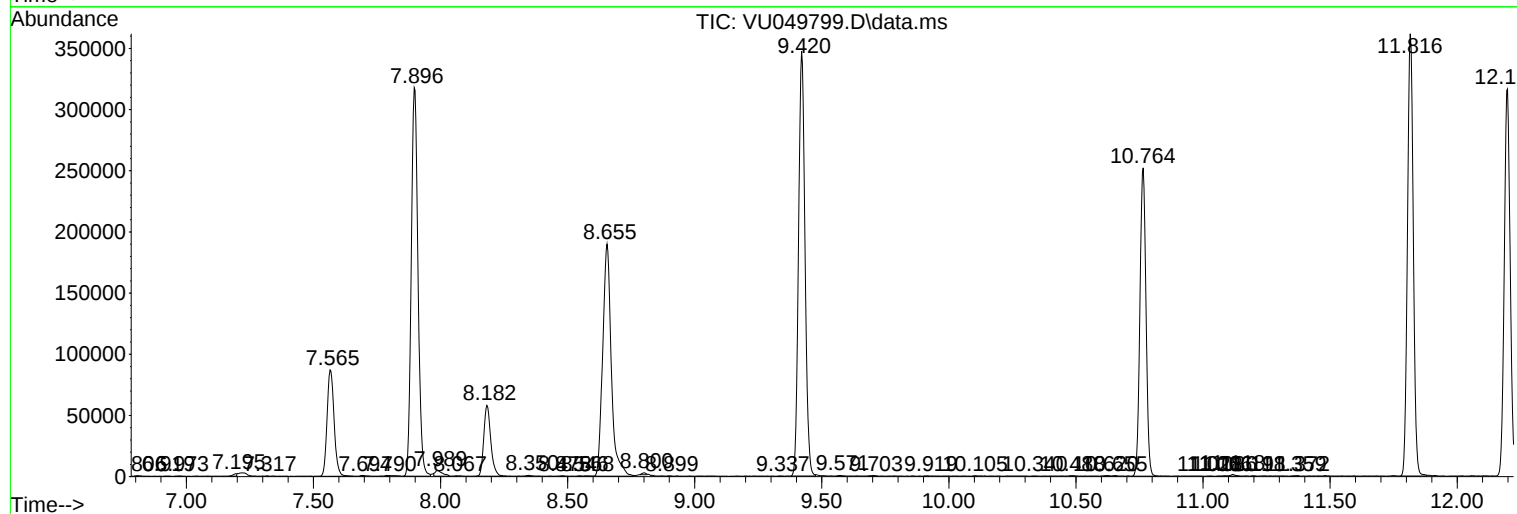
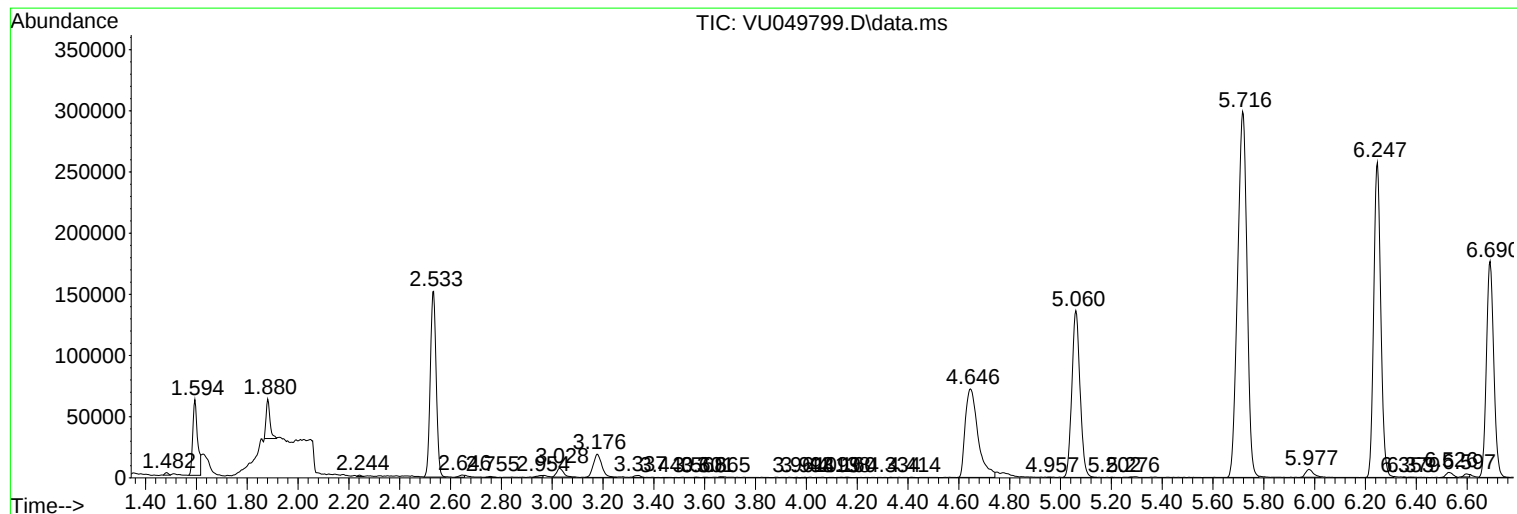
Sum of corrected areas: 6096462

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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
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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