

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071522\
 Data File : VU049742.D
 Acq On : 15 Jul 2022 17:22
 Operator : SY/MD
 Sample : N3679-14ME
 Misc : 6.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B54ME

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: VU049742.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	39	44	49	rBV3	2204	2203	0.11%	0.016%
2	1.514	49	54	66	rVB2	2708	3735	0.19%	0.027%
3	1.594	70	79	87	rBV	101542	148233	7.48%	1.082%
4	1.883	163	169	177	rBV	72936	97690	4.93%	0.713%
5	2.527	356	369	388	rVB	317623	510779	25.77%	3.727%
6	2.597	388	391	392	rBV	396	231	0.01%	0.002%
7	2.642	401	405	409	rBV4	1123	1249	0.06%	0.009%
8	2.916	487	490	491	rBV	276	137	0.01%	0.001%
9	2.954	497	502	506	rBV3	445	510	0.03%	0.004%
10	3.028	515	525	540	rBV3	6127	12090	0.61%	0.088%
11	3.179	558	572	584	rBV3	4799	11328	0.57%	0.083%
12	3.658	717	721	722	rBV2	490	274	0.01%	0.002%
13	4.530	989	992	996	rBV2	209	181	0.01%	0.001%
14	4.636	1012	1025	1069	rBV	227193	752989	38.00%	5.494%
15	4.903	1106	1108	1115	rVB2	657	476	0.02%	0.003%
16	5.060	1139	1157	1185	rBV	375873	857278	43.26%	6.255%
17	5.195	1196	1199	1203	rBV3	216	211	0.01%	0.002%
18	5.282	1221	1226	1227	rBV2	663	383	0.02%	0.003%
19	5.340	1241	1244	1247	rBV	236	151	0.01%	0.001%
20	5.369	1247	1253	1260	rVV4	769	975	0.05%	0.007%
21	5.481	1282	1288	1292	rBV2	422	492	0.02%	0.004%
22	5.565	1311	1314	1316	rBV	213	142	0.01%	0.001%
23	5.716	1340	1361	1391	rVV2	771603	1981789	100.00%	14.459%
24	5.980	1431	1443	1458	rBV3	7737	18220	0.92%	0.133%
25	6.118	1482	1486	1490	rVV3	235	228	0.01%	0.002%
26	6.243	1510	1525	1546	rVV	227398	447729	22.59%	3.267%
27	6.523	1603	1612	1627	rVV5	9467	17232	0.87%	0.126%
28	6.597	1627	1635	1648	rVV3	3077	6334	0.32%	0.046%
29	6.687	1648	1663	1687	rVV	492404	1002842	50.60%	7.317%
30	6.800	1695	1698	1701	rBV4	712	430	0.02%	0.003%
31	6.854	1714	1715	1719	rVB	437	155	0.01%	0.001%
32	7.131	1798	1801	1807	rVB2	174	157	0.01%	0.001%
33	7.189	1807	1819	1825	rBV3	6769	13766	0.69%	0.100%
34	7.311	1853	1857	1862	rVB3	492	390	0.02%	0.003%
35	7.337	1862	1865	1867	rBV	274	151	0.01%	0.001%
36	7.427	1890	1893	1896	rBV2	231	213	0.01%	0.002%

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

37	7.565	1923	1936	1961	rBV2	235402	440833	22.24%	3.216%
38	7.649	1961	1962	1964	rVV	529	211	0.01%	0.002%
39	7.694	1967	1976	1991	rVB3	4448	8951	0.45%	0.065%
40	7.764	1996	1998	2002	rBV	212	180	0.01%	0.001%
41	7.896	2025	2039	2061	rBV	809418	1413948	71.35%	10.316%
42	7.993	2061	2069	2084	rVB6	4729	10692	0.54%	0.078%
43	8.179	2113	2127	2155	rVV	155521	302347	15.26%	2.206%
44	8.298	2161	2164	2169	rVB2	411	318	0.02%	0.002%
45	8.340	2175	2177	2179	rBV	450	276	0.01%	0.002%
46	8.378	2187	2189	2193	rVB2	494	253	0.01%	0.002%
47	8.459	2213	2214	2220	rVB	215	168	0.01%	0.001%
48	8.568	2246	2248	2251	rBV	415	301	0.02%	0.002%
49	8.655	2257	2275	2309	rBV2	670441	1686849	85.12%	12.307%
50	8.800	2314	2320	2330	rVB5	3375	6296	0.32%	0.046%
51	8.883	2344	2346	2350	rVB2	427	245	0.01%	0.002%
52	8.912	2353	2355	2359	rVB2	219	138	0.01%	0.001%
53	8.941	2360	2364	2367	rVV3	465	287	0.01%	0.002%
54	8.964	2367	2371	2372	rVV3	205	171	0.01%	0.001%
55	9.015	2385	2387	2393	rVB2	286	186	0.01%	0.001%
56	9.047	2393	2397	2402	rBV2	258	274	0.01%	0.002%
57	9.185	2438	2440	2445	rVB	291	195	0.01%	0.001%
58	9.218	2445	2450	2456	rVB2	286	293	0.01%	0.002%
59	9.288	2466	2472	2475	rBV2	316	404	0.02%	0.003%
60	9.420	2499	2513	2534	rBV	303642	552606	27.88%	4.032%
61	9.574	2558	2561	2562	rBV	292	166	0.01%	0.001%
62	9.690	2591	2597	2599	rBV3	478	470	0.02%	0.003%
63	9.706	2599	2602	2605	rVB	346	257	0.01%	0.002%
64	9.902	2660	2663	2667	rVB2	247	202	0.01%	0.001%
65	9.928	2667	2671	2673	rBV2	293	274	0.01%	0.002%
66	10.073	2712	2716	2718	rBV	214	160	0.01%	0.001%
67	10.115	2724	2729	2731	rBV	301	266	0.01%	0.002%
68	10.246	2767	2770	2774	rBV	198	153	0.01%	0.001%
69	10.462	2835	2837	2846	rVB	264	255	0.01%	0.002%
70	10.542	2859	2862	2864	rBV2	234	171	0.01%	0.001%
71	10.645	2891	2894	2898	rBV4	425	351	0.02%	0.003%
72	10.684	2903	2906	2908	rBV2	268	174	0.01%	0.001%
73	10.761	2916	2930	2956	rBV	818866	1354632	68.35%	9.883%
74	11.073	3024	3027	3028	rBV2	261	164	0.01%	0.001%
75	11.118	3033	3041	3047	rVV4	1581	1995	0.10%	0.015%
76	11.285	3090	3093	3097	rBV	264	278	0.01%	0.002%

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 Title : VOC Analysis

77	11.308	3097	3100	3102	rVV2	251	139	0.01%	0.001%
78	11.369	3117	3119	3121	rBV	309	208	0.01%	0.002%
79	11.420	3132	3135	3140	rVB2	247	149	0.01%	0.001%
80	11.491	3153	3157	3161	rVB	304	216	0.01%	0.002%
81	11.562	3176	3179	3183	rBV2	303	242	0.01%	0.002%
82	11.584	3183	3186	3189	rVB	234	154	0.01%	0.001%
83	11.816	3244	3258	3271	rBV	322188	507685	25.62%	3.704%
84	11.989	3306	3312	3317	rVB3	348	456	0.02%	0.003%
85	12.137	3355	3358	3361	rBV2	186	150	0.01%	0.001%
86	12.195	3363	3376	3392	rBV	953610	1514874	76.44%	11.052%
87	12.394	3434	3438	3441	rBV2	520	456	0.02%	0.003%
88	12.410	3441	3443	3445	rBV2	272	156	0.01%	0.001%
89	12.816	3565	3569	3575	rBV2	313	256	0.01%	0.002%
90	13.025	3630	3634	3635	rBV	309	221	0.01%	0.002%
91	13.488	3775	3778	3781	rBB	277	153	0.01%	0.001%
92	13.822	3880	3882	3889	rVB2	341	300	0.02%	0.002%
93	13.854	3889	3892	3894	rBV2	415	225	0.01%	0.002%
94	13.989	3930	3934	3936	rBV	368	290	0.01%	0.002%
95	14.529	4100	4102	4105	rBV	286	164	0.01%	0.001%
96	14.664	4141	4144	4145	rBV	284	168	0.01%	0.001%
97	14.674	4145	4147	4151	rVV3	306	181	0.01%	0.001%
98	14.854	4201	4203	4205	rBV2	318	172	0.01%	0.001%
99	14.899	4211	4217	4220	rBV2	511	616	0.03%	0.004%
100	16.420	4687	4690	4697	rVB7	878	790	0.04%	0.006%

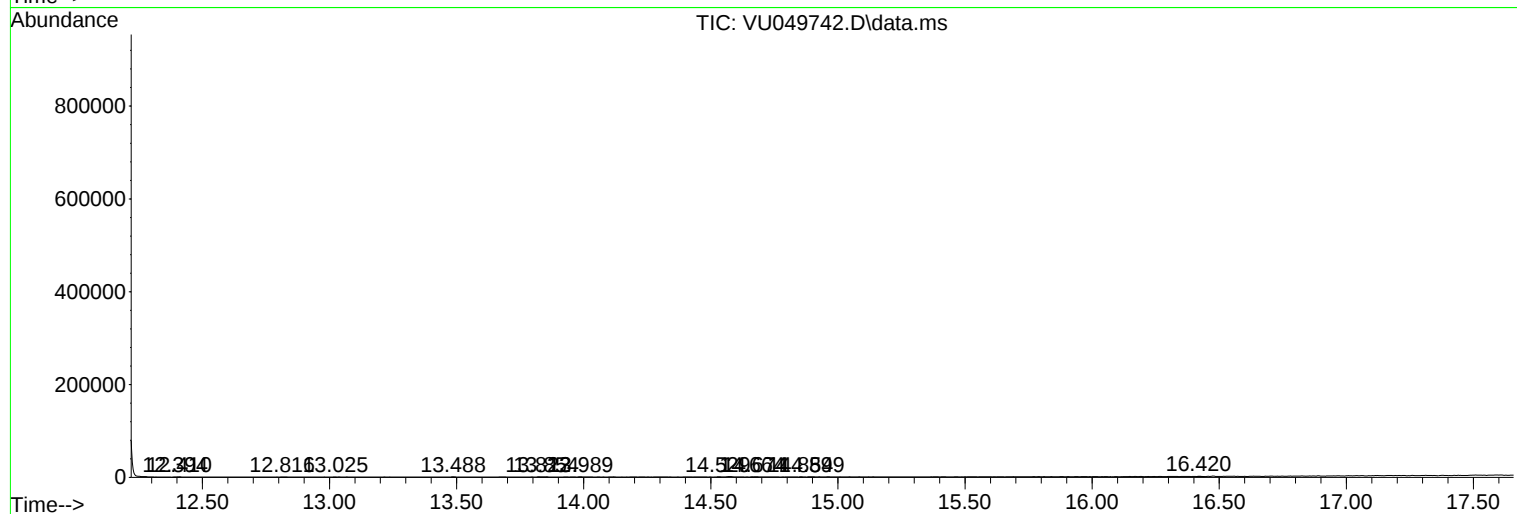
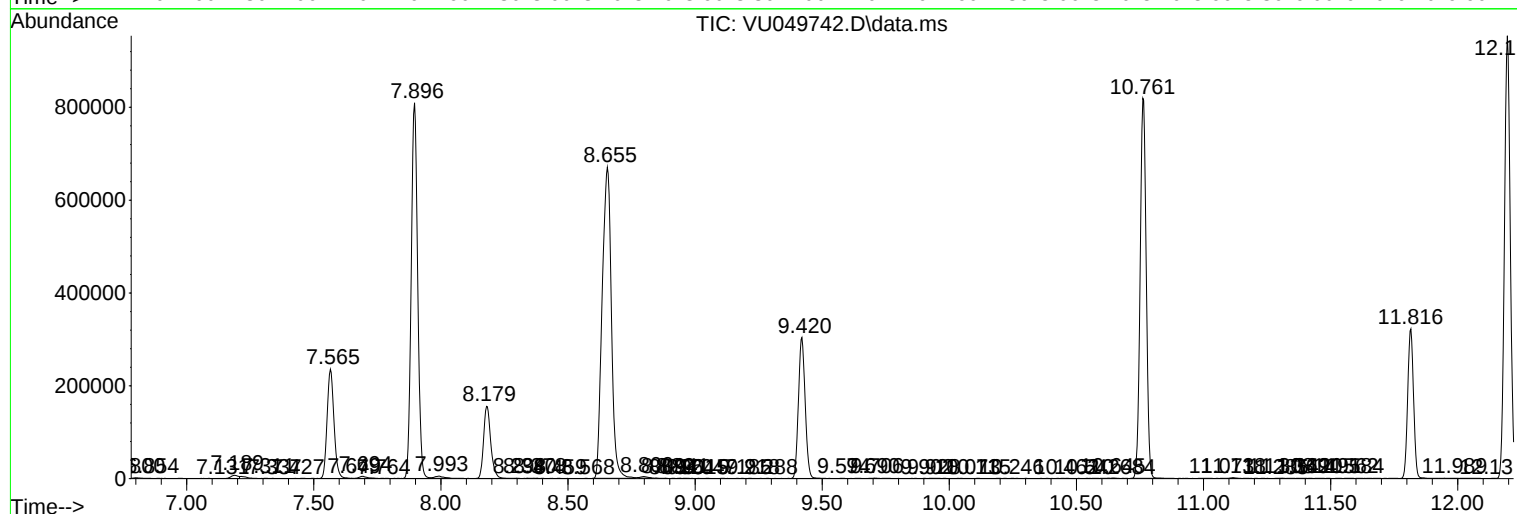
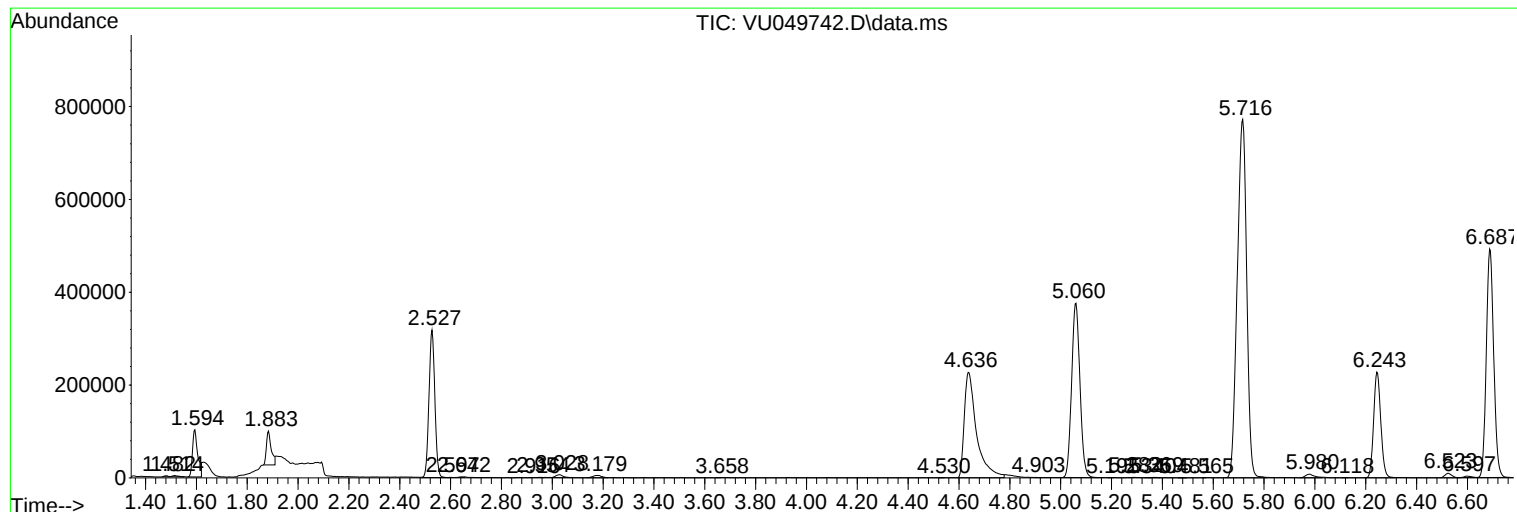
Sum of corrected areas: 13706184

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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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Instrument :
MSVOA_U
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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	--Internal Standard--			
					#	RT	Resp	Conc
