

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011122\
 Data File : VU046728.D
 Acq On : 11 Jan 2022 16:12
 Operator : SY/MD
 Sample : N1074-03ME
 Misc : 6.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGLK2ME

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\SFAMULM010522WMA.M
 Title : VOC Analysis

Signal : TIC: VU046728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	103	rVB	55243	68033	12.03%	1.315%
2	1.887	163	170	174	rBV	7251	9668	1.71%	0.187%
3	1.919	174	180	206	rVB	46271	67961	12.02%	1.314%
4	2.070	223	227	229	rBV	384	302	0.05%	0.006%
5	2.186	261	263	271	rVB	439	274	0.05%	0.005%
6	2.237	277	279	281	rBV2	271	189	0.03%	0.004%
7	2.449	343	345	352	rVB	263	177	0.03%	0.003%
8	2.568	371	382	395	rBV	96377	158507	28.03%	3.064%
9	2.790	449	451	455	rVB2	219	176	0.03%	0.003%
10	2.851	467	470	473	rVB	187	149	0.03%	0.003%
11	2.870	474	476	479	rBV	146	126	0.02%	0.002%
12	2.912	486	489	493	rBB	139	138	0.02%	0.003%
13	2.967	502	506	508	rBV2	277	226	0.04%	0.004%
14	2.983	508	511	514	rVB	281	244	0.04%	0.005%
15	3.051	528	532	537	rBV3	551	653	0.12%	0.013%
16	3.189	563	575	587	rBV2	3224	7158	1.27%	0.138%
17	3.825	769	773	775	rBB	177	133	0.02%	0.003%
18	3.877	786	789	793	rBB	276	197	0.03%	0.004%
19	4.652	1014	1030	1072	rBV	59817	227316	40.20%	4.394%
20	4.899	1105	1107	1111	rVB	201	134	0.02%	0.003%
21	4.993	1135	1136	1140	rBB	231	127	0.02%	0.002%
22	5.067	1143	1159	1183	rBV2	115184	251217	44.43%	4.856%
23	5.173	1190	1192	1197	rVB	135	140	0.02%	0.003%
24	5.726	1343	1364	1388	rBV2	204908	565478	100.00%	10.930%
25	5.980	1438	1443	1445	rBV2	472	442	0.08%	0.009%
26	6.250	1513	1527	1549	rBV	206335	389112	68.81%	7.521%
27	6.388	1568	1570	1573	rBB	169	115	0.02%	0.002%
28	6.536	1609	1616	1619	rVB2	642	780	0.14%	0.015%
29	6.607	1635	1638	1640	rBV2	257	180	0.03%	0.003%
30	6.623	1641	1643	1646	rVB2	213	113	0.02%	0.002%
31	6.693	1651	1665	1688	rBV	137452	269200	47.61%	5.203%
32	6.809	1699	1701	1704	rVB	284	140	0.02%	0.003%
33	7.031	1767	1770	1773	rBV	123	133	0.02%	0.003%
34	7.054	1773	1777	1781	rVB	314	268	0.05%	0.005%
35	7.192	1812	1820	1826	rBB3	680	928	0.16%	0.018%
36	7.568	1925	1937	1954	rBV	73393	128527	22.73%	2.484%

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 Title : VOC Analysis

37	7.697	1970	1977	1980	rBV2	347	519	0.09%	0.010%
38	7.710	1980	1981	1984	rVB	287	152	0.03%	0.003%
39	7.783	2001	2004	2005	rBV	279	156	0.03%	0.003%
40	7.793	2005	2007	2012	rVB	435	349	0.06%	0.007%
41	7.899	2027	2040	2055	rBV	233027	400121	70.76%	7.734%
42	8.182	2115	2128	2145	rBV2	53697	91876	16.25%	1.776%
43	8.263	2149	2153	2155	rVB2	324	241	0.04%	0.005%
44	8.288	2158	2161	2164	rBB	141	124	0.02%	0.002%
45	8.472	2216	2218	2223	rBB	254	185	0.03%	0.004%
46	8.571	2245	2249	2251	rBV	163	150	0.03%	0.003%
47	8.648	2258	2273	2298	rBV	247426	498653	88.18%	9.638%
48	8.796	2316	2319	2321	rBV	191	128	0.02%	0.002%
49	8.912	2353	2355	2357	rBV	239	148	0.03%	0.003%
50	8.980	2373	2376	2379	rBB	132	113	0.02%	0.002%
51	9.057	2398	2400	2405	rBB	146	151	0.03%	0.003%
52	9.243	2455	2458	2460	rBV	157	134	0.02%	0.003%
53	9.359	2492	2494	2498	rBV	155	154	0.03%	0.003%
54	9.420	2500	2513	2533	rBV	301148	502567	88.87%	9.714%
55	9.616	2570	2574	2576	rBV	155	152	0.03%	0.003%
56	9.677	2590	2593	2596	rBB	141	120	0.02%	0.002%
57	9.700	2596	2600	2602	rBB2	231	157	0.03%	0.003%
58	9.729	2607	2609	2612	rBV	137	115	0.02%	0.002%
59	9.754	2614	2617	2621	rBB	145	148	0.03%	0.003%
60	9.793	2625	2629	2631	rBV	150	148	0.03%	0.003%
61	10.066	2711	2714	2717	rBV	152	156	0.03%	0.003%
62	10.182	2747	2750	2753	rBV	174	160	0.03%	0.003%
63	10.394	2810	2816	2818	rBV	123	151	0.03%	0.003%
64	10.455	2830	2835	2837	rBB	137	140	0.02%	0.003%
65	10.513	2849	2853	2858	rBV	158	235	0.04%	0.005%
66	10.664	2897	2900	2904	rVV2	223	196	0.03%	0.004%
67	10.761	2915	2930	2946	rBV	297249	477540	84.45%	9.230%
68	10.819	2946	2948	2952	rVB	140	125	0.02%	0.002%
69	10.851	2955	2958	2960	rBV	155	131	0.02%	0.003%
70	10.893	2968	2971	2977	rBV2	203	175	0.03%	0.003%
71	10.976	2991	2997	3000	rBV	157	233	0.04%	0.005%
72	11.050	3017	3020	3023	rBV	126	132	0.02%	0.003%
73	11.108	3035	3038	3040	rBV	137	119	0.02%	0.002%
74	11.137	3043	3047	3049	rBB	147	120	0.02%	0.002%
75	11.166	3053	3056	3060	rBB	149	122	0.02%	0.002%
76	11.243	3075	3080	3084	rBV	164	250	0.04%	0.005%

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 Title : VOC Analysis

77	11.304	3095	3099	3101	rBV	142	141	0.02%	0.003%
78	11.391	3123	3126	3131	rBB	129	159	0.03%	0.003%
79	11.417	3132	3134	3137	rBV	129	116	0.02%	0.002%
80	11.475	3148	3152	3156	rVB	256	237	0.04%	0.005%
81	11.742	3231	3235	3237	rBV	141	119	0.02%	0.002%
82	11.812	3245	3257	3275	rVV	317894	498582	88.17%	9.637%
83	11.967	3303	3305	3309	rVB	145	116	0.02%	0.002%
84	12.195	3363	3376	3393	rVV	346213	545316	96.43%	10.540%
85	12.455	3451	3457	3460	rBV	208	273	0.05%	0.005%
86	12.770	3551	3555	3561	rBV2	201	277	0.05%	0.005%
87	12.992	3617	3624	3627	rBV	198	321	0.06%	0.006%
88	13.256	3703	3706	3711	rBV	101	115	0.02%	0.002%
89	13.552	3792	3798	3801	rBV	132	158	0.03%	0.003%
90	14.198	3996	3999	4007	rVB	145	152	0.03%	0.003%
91	14.571	4112	4115	4122	rBV2	289	348	0.06%	0.007%
92	15.233	4318	4321	4323	rBV2	182	136	0.02%	0.003%
93	15.307	4341	4344	4352	rBV2	216	256	0.05%	0.005%
94	15.610	4433	4438	4440	rBV2	233	263	0.05%	0.005%
95	15.635	4443	4446	4449	rVV2	184	135	0.02%	0.003%
96	15.703	4464	4467	4470	rBV	167	163	0.03%	0.003%
97	15.986	4549	4555	4558	rBV2	245	343	0.06%	0.007%
98	16.191	4616	4619	4623	rBV2	264	231	0.04%	0.004%
99	16.381	4675	4678	4682	rBV	288	205	0.04%	0.004%
100	17.124	4907	4909	4911	rBV2	419	187	0.03%	0.004%

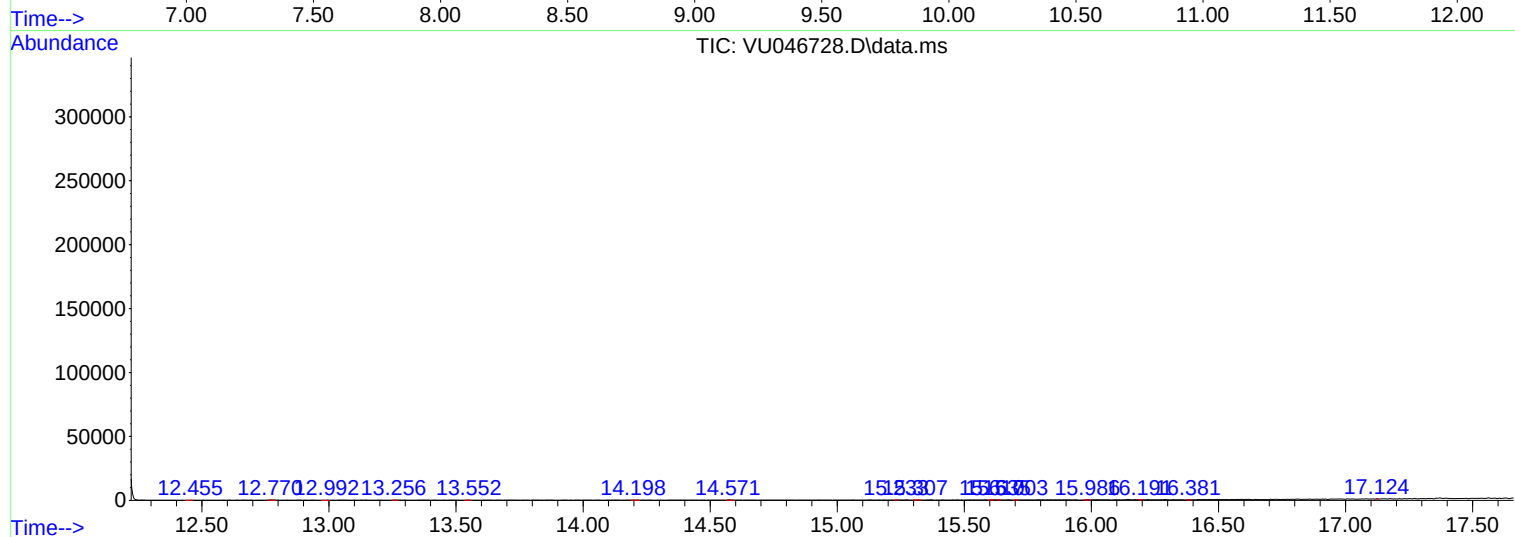
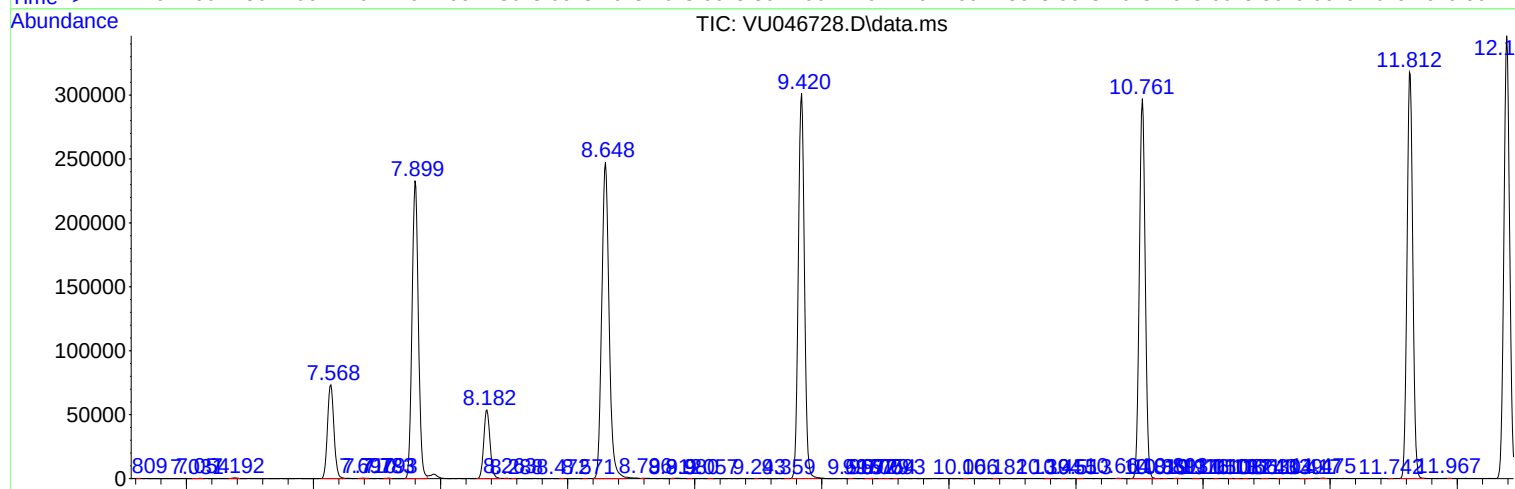
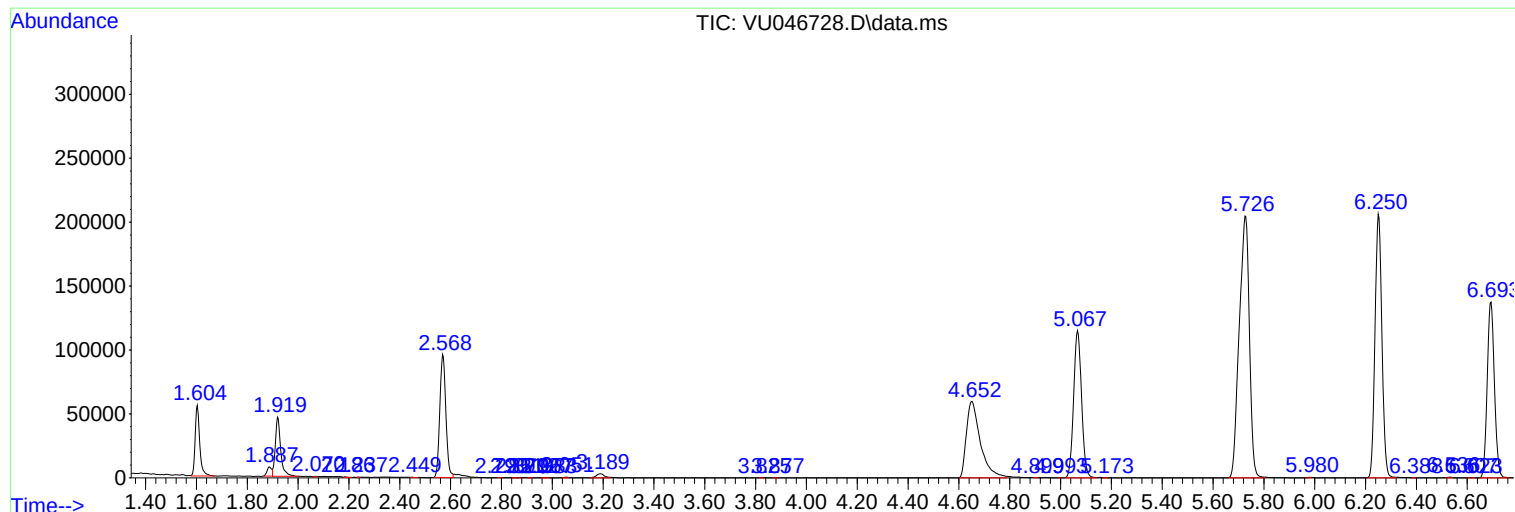
Sum of corrected areas: 5173756

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM010522WMA.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\SFAMULM010522WMA.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