

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121521\
 Data File : VU046402.D
 Acq On : 15 Dec 2021 17:39
 Operator : SY/MD
 Sample : M5023-20MEDL 10X
 Misc : 6.26g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGKZ8MEDL

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046402.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	73	82	103	rVB	64077	80718	16.68%	1.825%
2	1.887	161	170	174	rBV	12488	17067	3.53%	0.386%
3	1.919	174	180	199	rVB	42967	61073	12.62%	1.381%
4	2.031	213	215	219	rBV	531	346	0.07%	0.008%
5	2.366	317	319	323	rBV2	233	210	0.04%	0.005%
6	2.572	370	383	404	rBV	107773	180475	37.30%	4.080%
7	2.748	436	438	441	rBV	129	115	0.02%	0.003%
8	2.909	485	488	490	rBV	140	121	0.03%	0.003%
9	2.957	500	503	505	rBV	242	174	0.04%	0.004%
10	3.002	512	517	520	rBB	146	173	0.04%	0.004%
11	3.054	526	533	540	rVV2	632	803	0.17%	0.018%
12	3.186	565	574	588	rBB3	1872	4198	0.87%	0.095%
13	3.456	653	658	660	rBB	131	137	0.03%	0.003%
14	3.629	709	712	715	rBB	132	115	0.02%	0.003%
15	3.877	777	789	799	rBV3	2045	4017	0.83%	0.091%
16	4.044	838	841	843	rBV	139	118	0.02%	0.003%
17	4.639	1012	1026	1052	rBV2	39247	111580	23.06%	2.522%
18	4.970	1125	1129	1131	rBB	144	118	0.02%	0.003%
19	5.067	1144	1159	1182	rBV	88447	191008	39.48%	4.318%
20	5.147	1182	1184	1187	rVB	267	171	0.04%	0.004%
21	5.166	1187	1190	1194	rBB	248	187	0.04%	0.004%
22	5.186	1194	1196	1198	rBV	168	119	0.02%	0.003%
23	5.215	1203	1205	1209	rVV	174	129	0.03%	0.003%
24	5.234	1209	1211	1216	rVB2	235	177	0.04%	0.004%
25	5.729	1344	1365	1383	rBV2	181166	483827	100.00%	10.937%
26	5.973	1438	1441	1445	rBB2	241	179	0.04%	0.004%
27	6.250	1514	1527	1549	rBV	184103	346811	71.68%	7.840%
28	6.327	1549	1551	1559	rVV2	328	380	0.08%	0.009%
29	6.546	1607	1619	1631	rBB	25748	47160	9.75%	1.066%
30	6.694	1650	1665	1686	rBV	110815	212727	43.97%	4.809%
31	6.864	1713	1718	1722	rBB	140	198	0.04%	0.004%
32	6.893	1723	1727	1730	rBV	142	140	0.03%	0.003%
33	7.044	1772	1774	1775	rBV	221	126	0.03%	0.003%
34	7.185	1814	1818	1820	rBV	259	229	0.05%	0.005%
35	7.568	1925	1937	1955	rBV	58798	101800	21.04%	2.301%
36	7.674	1966	1970	1974	rBB	126	133	0.03%	0.003%

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 Title : VOC Analysis

37	7.706	1977	1980	1984	rBB	140	146	0.03%	0.003%
38	7.790	2000	2006	2014	rBV3	646	1036	0.21%	0.023%
39	7.899	2027	2040	2056	rBV	222856	382875	79.13%	8.655%
40	8.179	2116	2127	2143	rBV	42028	68278	14.11%	1.543%
41	8.275	2154	2157	2161	rBV2	134	158	0.03%	0.004%
42	8.314	2166	2169	2173	rBB	158	160	0.03%	0.004%
43	8.356	2178	2182	2185	rBV	154	180	0.04%	0.004%
44	8.475	2210	2219	2227	rBV2	1417	2348	0.49%	0.053%
45	8.555	2228	2244	2258	rVV	228852	383507	79.27%	8.669%
46	8.636	2258	2269	2291	rVV	135228	236116	48.80%	5.337%
47	8.726	2294	2297	2300	rBV2	178	165	0.03%	0.004%
48	8.800	2316	2320	2321	rBV	144	120	0.02%	0.003%
49	8.922	2347	2358	2366	rBV3	853	1495	0.31%	0.034%
50	8.980	2374	2376	2380	rBB	139	116	0.02%	0.003%
51	9.066	2398	2403	2405	rBV	147	174	0.04%	0.004%
52	9.166	2430	2434	2437	rBB	187	170	0.04%	0.004%
53	9.214	2447	2449	2452	rBV	151	128	0.03%	0.003%
54	9.256	2459	2462	2466	rBV	146	176	0.04%	0.004%
55	9.279	2466	2469	2474	rVV	100	119	0.02%	0.003%
56	9.337	2485	2487	2491	rBV	140	141	0.03%	0.003%
57	9.417	2497	2512	2532	rBV	270874	444462	91.86%	10.047%
58	9.539	2546	2550	2556	rBV	186	270	0.06%	0.006%
59	9.619	2570	2575	2578	rBB	166	157	0.03%	0.004%
60	9.697	2595	2599	2602	rBV	434	333	0.07%	0.008%
61	9.748	2609	2615	2620	rBV	165	310	0.06%	0.007%
62	10.066	2711	2714	2719	rBV	171	209	0.04%	0.005%
63	10.201	2751	2756	2758	rBB	133	115	0.02%	0.003%
64	10.253	2768	2772	2775	rBV	163	184	0.04%	0.004%
65	10.295	2780	2785	2791	rBB	174	270	0.06%	0.006%
66	10.340	2794	2799	2804	rBV	211	302	0.06%	0.007%
67	10.423	2821	2825	2826	rBV	155	133	0.03%	0.003%
68	10.488	2842	2845	2847	rBV	155	126	0.03%	0.003%
69	10.674	2895	2903	2909	rVB3	1003	1271	0.26%	0.029%
70	10.758	2917	2929	2946	rVB	158286	251218	51.92%	5.679%
71	10.899	2964	2973	2985	rBV3	731	1476	0.31%	0.033%
72	11.050	3015	3020	3023	rBV	181	219	0.05%	0.005%
73	11.192	3058	3064	3073	rBB	204	424	0.09%	0.010%
74	11.311	3096	3101	3102	rBV	151	156	0.03%	0.004%
75	11.356	3112	3115	3117	rBV	140	126	0.03%	0.003%
76	11.462	3145	3148	3156	rVB2	792	802	0.17%	0.018%

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77	11.581	3181	3185	3189	rBV	186	222	0.05%	0.005%
78	11.668	3206	3212	3214	rBV	189	223	0.05%	0.005%
79	11.690	3215	3219	3222	rBV3	267	256	0.05%	0.006%
80	11.812	3245	3257	3277	rVV	290988	448692	92.74%	10.143%
81	11.941	3293	3297	3300	rBV	219	200	0.04%	0.005%
82	11.973	3300	3307	3313	rVV2	595	837	0.17%	0.019%
83	12.195	3364	3376	3391	rVB	214433	342051	70.70%	7.732%
84	12.320	3412	3415	3421	rBB	167	214	0.04%	0.005%
85	12.362	3422	3428	3432	rBV	197	310	0.06%	0.007%
86	12.774	3551	3556	3562	rVB2	467	602	0.12%	0.014%
87	12.947	3607	3610	3616	rBV	123	118	0.02%	0.003%
88	13.233	3695	3699	3706	rBV	111	127	0.03%	0.003%
89	13.430	3755	3760	3763	rBV	139	132	0.03%	0.003%
90	14.574	4111	4116	4118	rBV	331	333	0.07%	0.008%
91	15.349	4354	4357	4363	rVB2	188	196	0.04%	0.004%
92	15.475	4393	4396	4400	rBV	208	128	0.03%	0.003%
93	15.613	4433	4439	4441	rBV2	256	348	0.07%	0.008%
94	15.684	4459	4461	4465	rBV2	161	115	0.02%	0.003%
95	15.864	4514	4517	4522	rBV2	263	275	0.06%	0.006%
96	16.034	4567	4570	4572	rBV	222	180	0.04%	0.004%
97	16.497	4711	4714	4717	rBV	332	207	0.04%	0.005%
98	16.716	4779	4782	4783	rBV	287	168	0.03%	0.004%
99	16.931	4847	4849	4854	rVB2	317	187	0.04%	0.004%
100	17.053	4884	4887	4890	rBV2	458	384	0.08%	0.009%

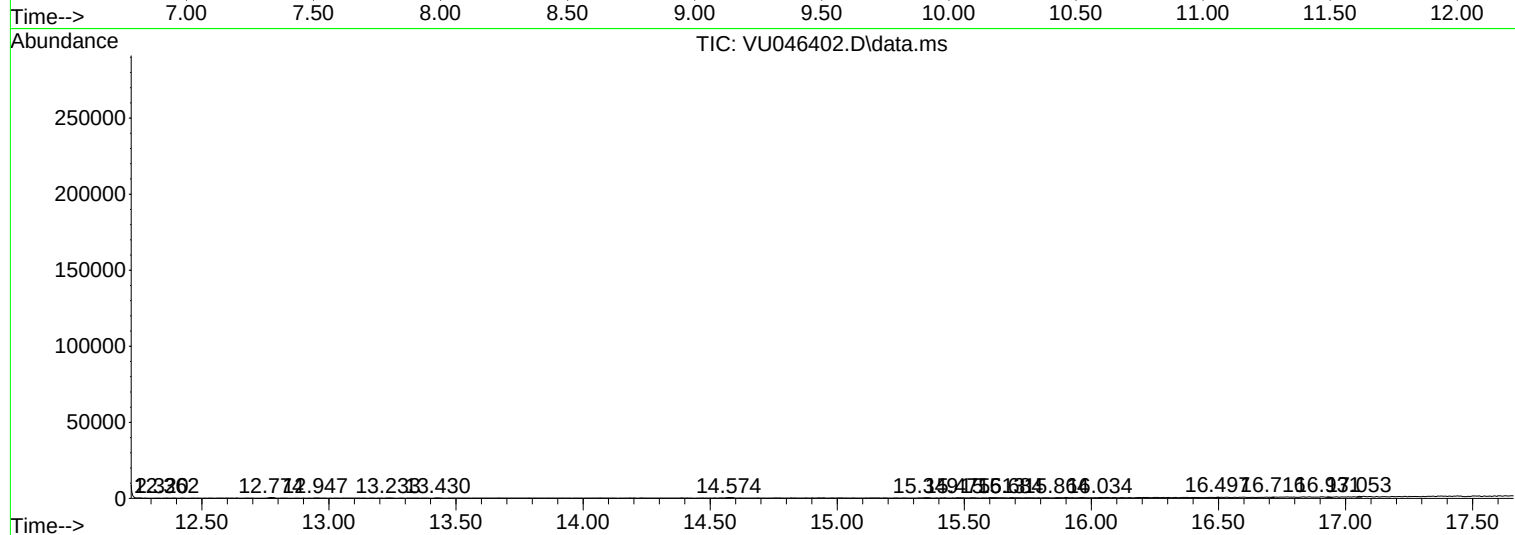
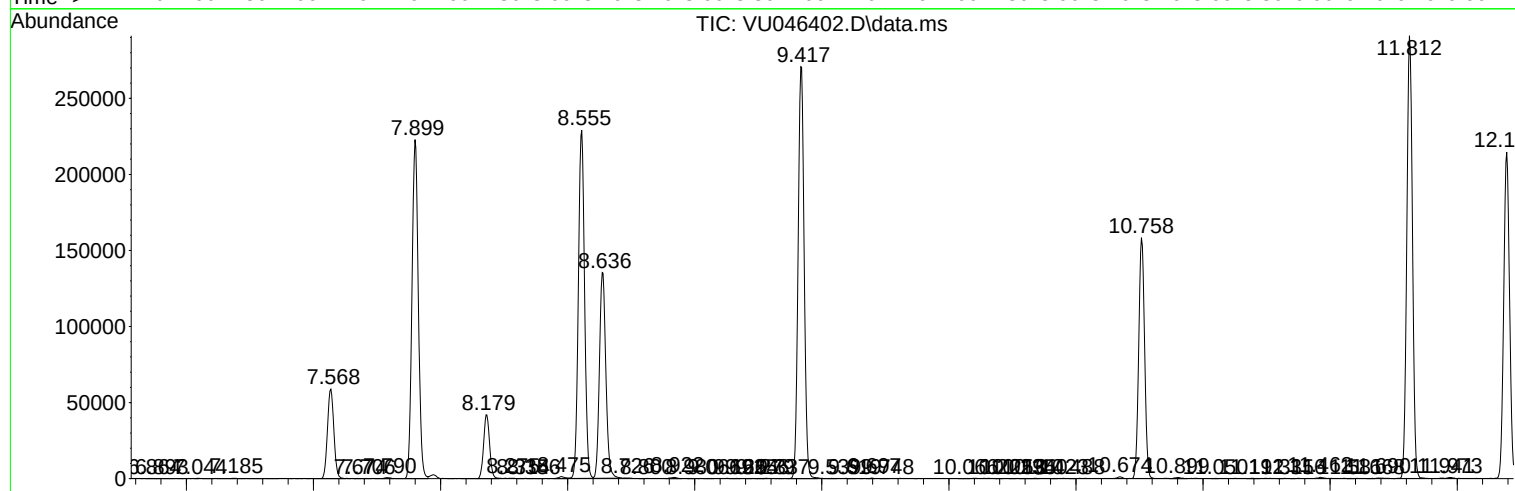
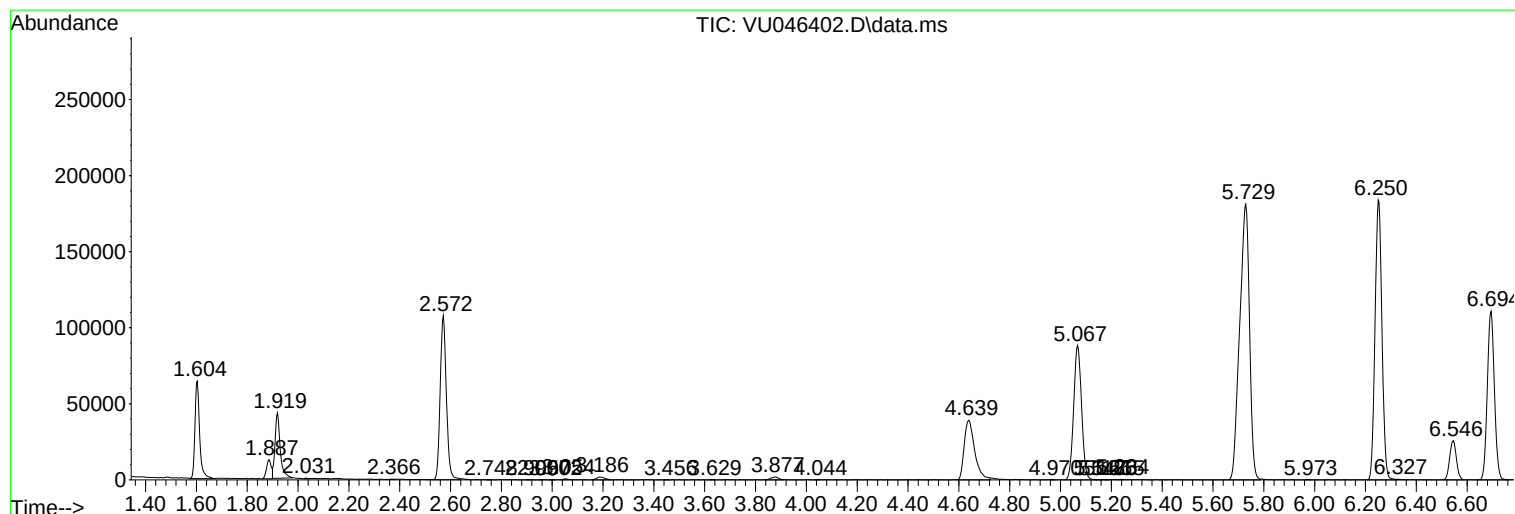
Sum of corrected areas: 4423735

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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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	--Internal Standard--			
					#	RT	Resp	Conc