

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046129.D
 Acq On : 07 Dec 2021 10:53
 Operator : SY/MD
 Sample : VU1207MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 28 Sample Multiplier: 1

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: VU046129.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	95	rBV	145002	161887	15.42%	2.003%
2	1.919	171	180	193	rBV	103514	132368	12.61%	1.638%
3	2.501	359	361	362	rBV	275	147	0.01%	0.002%
4	2.575	371	384	410	rBV	236990	398659	37.97%	4.934%
5	2.697	419	422	425	rBV2	333	248	0.02%	0.003%
6	2.768	442	444	447	rVV2	289	156	0.01%	0.002%
7	2.800	447	454	463	rVV2	903	1466	0.14%	0.018%
8	2.967	499	506	510	rBV	294	394	0.04%	0.005%
9	3.054	524	533	539	rBV3	1115	1651	0.16%	0.020%
10	3.247	589	593	596	rBV	182	194	0.02%	0.002%
11	3.362	627	629	634	rVB	226	142	0.01%	0.002%
12	3.542	682	685	688	rBV	191	194	0.02%	0.002%
13	3.610	700	706	711	rBV	178	280	0.03%	0.003%
14	3.771	751	756	759	rBV	146	190	0.02%	0.002%
15	4.182	880	884	887	rBV	138	144	0.01%	0.002%
16	4.446	962	966	970	rBB	137	168	0.02%	0.002%
17	4.642	1011	1027	1073	rBV	82357	255623	24.34%	3.163%
18	4.906	1104	1109	1115	rVB2	319	341	0.03%	0.004%
19	5.070	1142	1160	1185	rBV	178560	404227	38.50%	5.003%
20	5.272	1219	1223	1226	rBV2	425	399	0.04%	0.005%
21	5.295	1226	1230	1234	rVB3	504	407	0.04%	0.005%
22	5.571	1314	1316	1324	rBV	146	246	0.02%	0.003%
23	5.729	1343	1365	1386	rBV2	390264	1050012	100.00%	12.994%
24	5.938	1428	1430	1438	rVB	216	138	0.01%	0.002%
25	6.073	1470	1472	1476	rVB2	271	213	0.02%	0.003%
26	6.095	1476	1479	1482	rBV	202	183	0.02%	0.002%
27	6.115	1482	1485	1487	rVV	235	131	0.01%	0.002%
28	6.185	1503	1507	1511	rBB	166	182	0.02%	0.002%
29	6.253	1513	1528	1546	rBV	290835	544614	51.87%	6.740%
30	6.404	1573	1575	1579	rVB2	213	135	0.01%	0.002%
31	6.536	1606	1616	1625	rBV4	3445	6383	0.61%	0.079%
32	6.693	1651	1665	1686	rBV	231736	450248	42.88%	5.572%
33	6.800	1696	1698	1699	rBV2	390	174	0.02%	0.002%
34	6.812	1700	1702	1708	rVB5	924	836	0.08%	0.010%
35	6.883	1721	1724	1727	rBV	149	151	0.01%	0.002%
36	7.041	1769	1773	1780	rVB2	354	366	0.03%	0.005%

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 ALS Vial : 28 Sample Multiplier: 1

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

37	7.131	1799	1801	1803	rBV	263	146	0.01%	0.002%
38	7.189	1813	1819	1824	rVB3	617	741	0.07%	0.009%
39	7.246	1834	1837	1840	rBV	196	168	0.02%	0.002%
40	7.568	1924	1937	1958	rBV	139692	240947	22.95%	2.982%
41	7.719	1980	1984	1987	rVB2	278	183	0.02%	0.002%
42	7.793	2002	2007	2012	rBV2	245	367	0.03%	0.005%
43	7.902	2027	2041	2057	rBV	514197	894583	85.20%	11.071%
44	8.182	2115	2128	2142	rBV2	94606	157257	14.98%	1.946%
45	8.465	2214	2216	2220	rVB2	186	152	0.01%	0.002%
46	8.510	2227	2230	2233	rBV	137	138	0.01%	0.002%
47	8.568	2246	2248	2251	rBV	174	150	0.01%	0.002%
48	8.635	2256	2269	2301	rVV	295113	525544	50.05%	6.504%
49	8.799	2316	2320	2322	rBV2	213	153	0.01%	0.002%
50	8.989	2376	2379	2384	rVB2	272	262	0.02%	0.003%
51	9.163	2427	2433	2439	rBV3	663	827	0.08%	0.010%
52	9.420	2499	2513	2549	rVB	413253	686195	65.35%	8.492%
53	9.571	2554	2560	2570	rBV3	642	1027	0.10%	0.013%
54	9.645	2578	2583	2589	rVV	176	238	0.02%	0.003%
55	9.697	2592	2599	2609	rVB2	1164	1674	0.16%	0.021%
56	10.115	2720	2729	2731	rBV2	767	1128	0.11%	0.014%
57	10.262	2772	2775	2779	rVB	181	182	0.02%	0.002%
58	10.298	2779	2786	2789	rBV2	423	399	0.04%	0.005%
59	10.488	2840	2845	2852	rBV2	643	780	0.07%	0.010%
60	10.674	2894	2903	2911	rBV3	2677	3826	0.36%	0.047%
61	10.761	2917	2930	2945	rBV	323328	533132	50.77%	6.598%
62	10.832	2950	2952	2957	rVV2	514	298	0.03%	0.004%
63	10.870	2957	2964	2968	rVV2	539	768	0.07%	0.010%
64	10.893	2969	2971	2977	rVV2	559	431	0.04%	0.005%
65	10.928	2977	2982	2987	rVB2	285	289	0.03%	0.004%
66	11.005	3002	3006	3009	rBV2	188	145	0.01%	0.002%
67	11.092	3026	3033	3039	rBV2	907	1442	0.14%	0.018%
68	11.121	3039	3042	3049	rVV2	643	584	0.06%	0.007%
69	11.205	3065	3068	3072	rVB	136	136	0.01%	0.002%
70	11.462	3139	3148	3159	rVB4	2654	4533	0.43%	0.056%
71	11.581	3180	3185	3190	rVB3	494	543	0.05%	0.007%
72	11.700	3216	3222	3229	rBV3	1309	1602	0.15%	0.020%
73	11.748	3230	3237	3245	rVV2	1162	1712	0.16%	0.021%
74	11.812	3245	3257	3280	rVB	465885	737500	70.24%	9.127%
75	11.915	3286	3289	3291	rBV2	194	158	0.02%	0.002%
76	11.944	3291	3298	3302	rVV2	1032	1250	0.12%	0.015%

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 ALS Vial : 28 Sample Multiplier: 1

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

77	11.973	3302	3307	3315	rVB3	2160	2596	0.25%	0.032%
78	12.060	3329	3334	3338	rBV	123	149	0.01%	0.002%
79	12.195	3360	3376	3394	rBV	522123	832553	79.29%	10.303%
80	12.282	3401	3403	3406	rVB	280	133	0.01%	0.002%
81	12.330	3414	3418	3424	rVB4	625	672	0.06%	0.008%
82	12.465	3458	3460	3465	rVB2	259	181	0.02%	0.002%
83	12.770	3552	3555	3560	rVB2	212	229	0.02%	0.003%
84	13.224	3690	3696	3703	rBV4	1988	2623	0.25%	0.032%
85	13.629	3819	3822	3826	rBV2	270	229	0.02%	0.003%
86	13.844	3881	3889	3897	rBV	3405	4904	0.47%	0.061%
87	14.089	3956	3965	3979	rVB	8013	12509	1.19%	0.155%
88	14.262	4015	4019	4024	rVB2	209	202	0.02%	0.002%
89	14.294	4028	4029	4032	rVV	258	152	0.01%	0.002%
90	14.333	4033	4041	4050	rVB3	4091	6049	0.58%	0.075%
91	14.500	4090	4093	4095	rBV3	293	195	0.02%	0.002%
92	14.571	4111	4115	4116	rBV2	499	336	0.03%	0.004%
93	14.712	4157	4159	4165	rBV2	244	302	0.03%	0.004%
94	14.754	4169	4172	4176	rBV2	350	291	0.03%	0.004%
95	14.880	4208	4211	4213	rBV2	300	201	0.02%	0.002%
96	14.918	4219	4223	4224	rBV2	223	161	0.02%	0.002%
97	14.941	4227	4230	4233	rBV	232	152	0.01%	0.002%
98	15.150	4292	4295	4299	rBV2	330	212	0.02%	0.003%
99	15.754	4480	4483	4487	rBV2	378	289	0.03%	0.004%
100	16.230	4629	4631	4634	rBV2	437	256	0.02%	0.003%

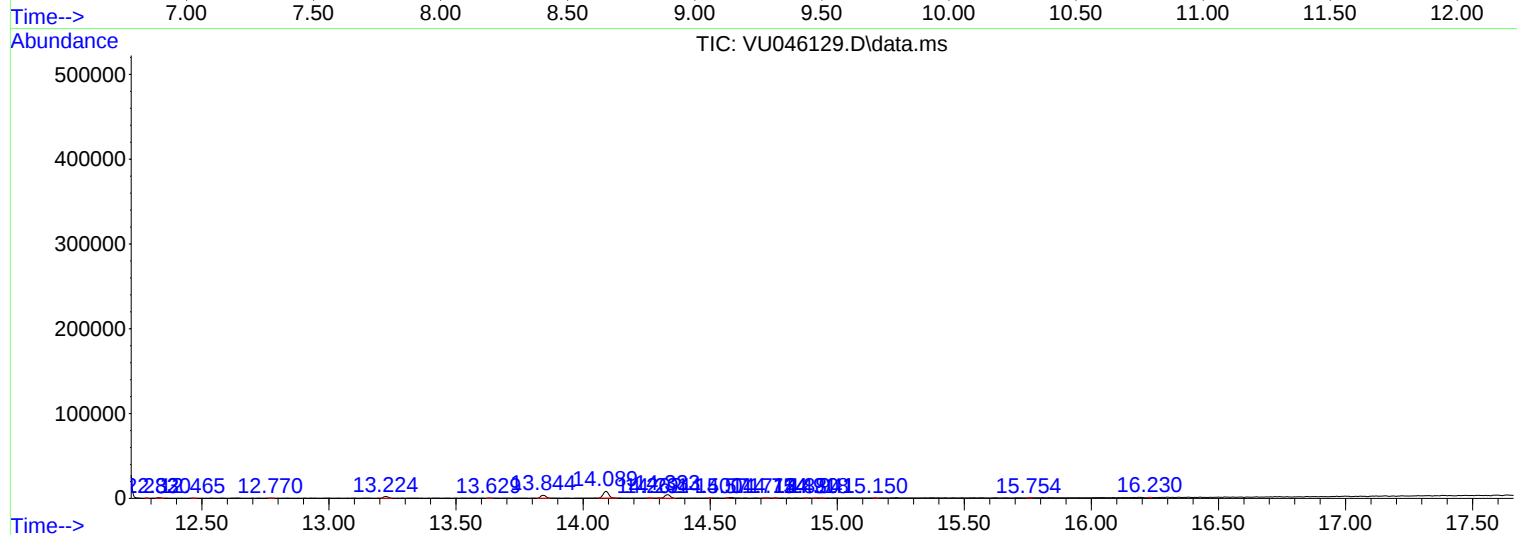
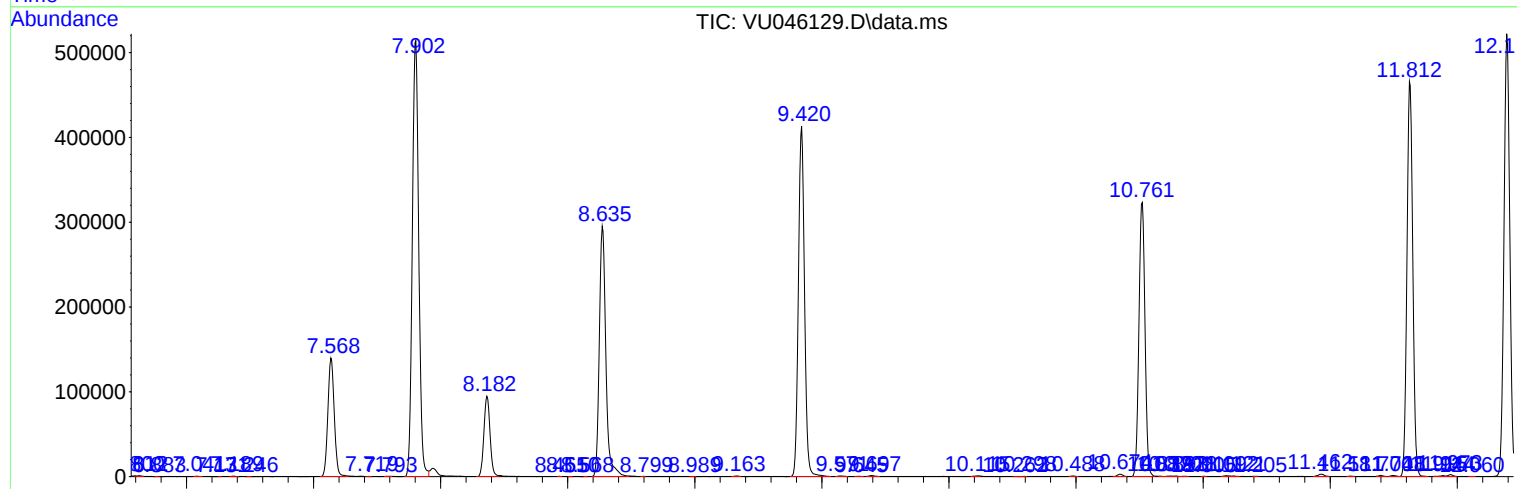
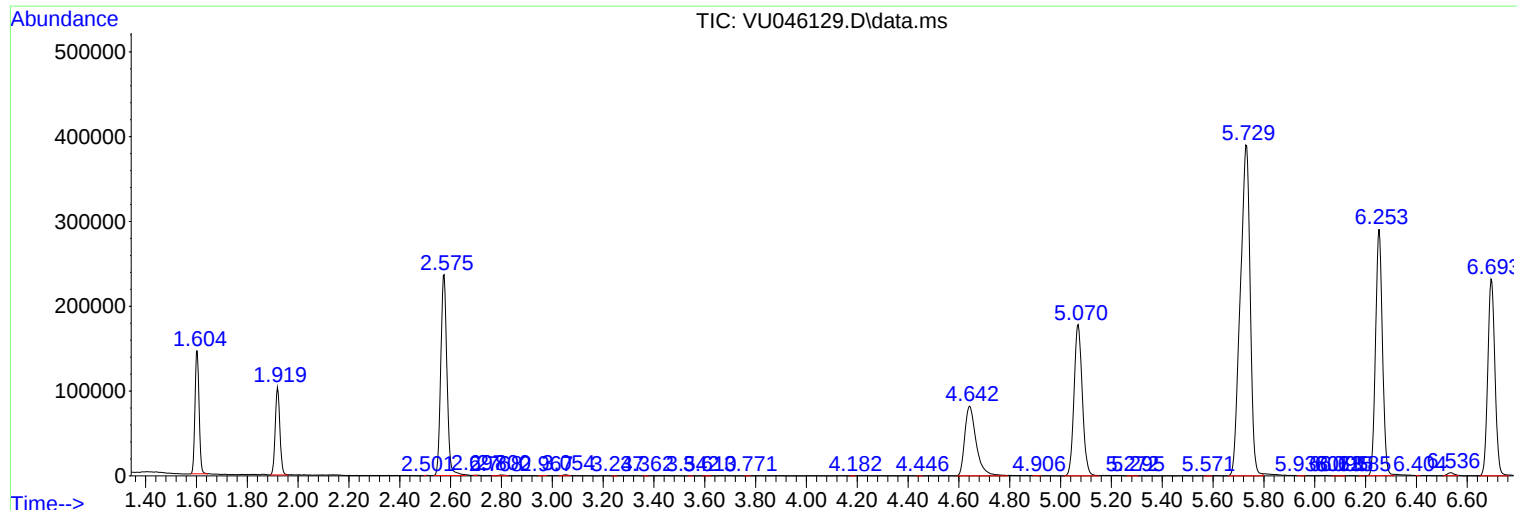
Sum of corrected areas: 8080463

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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
