

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083122\
 Data File : VU050563.D
 Acq On : 31 Aug 2022 20:53
 Operator : SY/MD
 Sample : N4363-16MERE
 Misc : 5.56g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVX0MERE

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\SFAMULM083022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050563.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	71	79	118	rBV	113398	182195	10.50%	1.559%
2	1.893	166	172	193	rBV	94488	136093	7.84%	1.164%
3	2.549	364	376	396	rBV	320420	514538	29.66%	4.402%
4	2.700	420	423	428	rVB3	504	382	0.02%	0.003%
5	2.732	428	433	437	rBV	337	300	0.02%	0.003%
6	2.755	438	440	443	rBV	169	114	0.01%	0.001%
7	2.819	457	460	463	rVB	272	222	0.01%	0.002%
8	2.867	472	475	478	rBV	206	126	0.01%	0.001%
9	2.925	490	493	501	rVB2	256	258	0.01%	0.002%
10	3.038	518	528	539	rBV2	2809	5001	0.29%	0.043%
11	3.176	559	571	589	rBV	4752	11452	0.66%	0.098%
12	3.356	624	627	632	rBV	255	140	0.01%	0.001%
13	3.430	648	650	653	rBV	187	104	0.01%	0.001%
14	3.475	661	664	666	rBV	182	130	0.01%	0.001%
15	3.543	683	685	689	rVB	192	97	0.01%	0.001%
16	3.616	705	708	713	rVV	267	172	0.01%	0.001%
17	3.661	719	722	727	rVB2	200	193	0.01%	0.002%
18	3.716	736	739	743	rVV	240	204	0.01%	0.002%
19	3.925	801	804	805	rBV	201	110	0.01%	0.001%
20	4.041	837	840	842	rVB	204	100	0.01%	0.001%
21	4.083	847	853	858	rBV2	170	165	0.01%	0.001%
22	4.108	858	861	866	rBB	168	109	0.01%	0.001%
23	4.137	867	870	872	rBV	198	98	0.01%	0.001%
24	4.221	890	896	899	rBV	194	207	0.01%	0.002%
25	4.433	957	962	964	rBV2	145	107	0.01%	0.001%
26	4.449	964	967	969	rVV2	169	108	0.01%	0.001%
27	4.542	993	996	999	rBV2	165	140	0.01%	0.001%
28	4.636	1008	1025	1071	rBV	138580	442583	25.51%	3.786%
29	5.060	1140	1157	1186	rBV	306190	676022	38.96%	5.783%
30	5.292	1221	1229	1232	rBV3	568	871	0.05%	0.007%
31	5.366	1248	1252	1255	rBV	290	300	0.02%	0.003%
32	5.507	1293	1296	1297	rBV	149	106	0.01%	0.001%
33	5.578	1314	1318	1321	rVB2	179	161	0.01%	0.001%
34	5.719	1341	1362	1396	rVV2	666219	1735004	100.00%	14.842%
35	5.983	1434	1444	1451	rBV7	1931	3808	0.22%	0.033%
36	6.028	1455	1458	1462	rVB3	390	313	0.02%	0.003%

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 Title : VOC Analysis

37	6.057	1462	1467	1469	rBV2	220	220	0.01%	0.002%
38	6.247	1510	1526	1547	rBV	378821	724687	41.77%	6.199%
39	6.475	1592	1597	1599	rBV2	279	297	0.02%	0.003%
40	6.520	1608	1611	1613	rBV2	1446	1078	0.06%	0.009%
41	6.603	1625	1637	1641	rBV4	997	1766	0.10%	0.015%
42	6.690	1649	1664	1693	rBV	400967	790233	45.55%	6.760%
43	6.931	1736	1739	1744	rVV2	175	160	0.01%	0.001%
44	6.983	1752	1755	1759	rVB2	183	115	0.01%	0.001%
45	7.009	1759	1763	1768	rVB2	236	188	0.01%	0.002%
46	7.144	1801	1805	1807	rBV2	135	110	0.01%	0.001%
47	7.192	1813	1820	1822	rBV3	948	975	0.06%	0.008%
48	7.459	1898	1903	1908	rVB2	211	241	0.01%	0.002%
49	7.484	1908	1911	1913	rBV	211	173	0.01%	0.001%
50	7.520	1919	1922	1923	rBV	156	110	0.01%	0.001%
51	7.565	1924	1936	1959	rVV	184427	329410	18.99%	2.818%
52	7.742	1989	1991	1994	rBV2	386	298	0.02%	0.003%
53	7.838	2016	2021	2025	rBV3	231	241	0.01%	0.002%
54	7.896	2025	2039	2061	rBV	782337	1348222	77.71%	11.533%
55	8.179	2116	2127	2146	rBV	127352	219572	12.66%	1.878%
56	8.327	2170	2173	2176	rBV	348	279	0.02%	0.002%
57	8.410	2195	2199	2203	rVB3	351	297	0.02%	0.003%
58	8.507	2227	2229	2232	rBV2	189	119	0.01%	0.001%
59	8.552	2235	2243	2252	rVB4	6287	9921	0.57%	0.085%
60	8.645	2258	2272	2304	rBV2	453772	971667	56.00%	8.312%
61	8.925	2354	2359	2365	rBV3	463	602	0.03%	0.005%
62	8.964	2369	2371	2373	rBV2	385	185	0.01%	0.002%
63	9.198	2441	2444	2448	rBV2	218	164	0.01%	0.001%
64	9.221	2448	2451	2453	rVV	217	149	0.01%	0.001%
65	9.243	2455	2458	2462	rVB	273	189	0.01%	0.002%
66	9.288	2469	2472	2474	rBV2	221	130	0.01%	0.001%
67	9.304	2474	2477	2483	rVB	308	303	0.02%	0.003%
68	9.333	2483	2486	2488	rBV	242	186	0.01%	0.002%
69	9.417	2496	2512	2533	rBV	516618	863178	49.75%	7.384%
70	9.603	2567	2570	2573	rVB	473	218	0.01%	0.002%
71	9.777	2621	2624	2625	rBV2	159	96	0.01%	0.001%
72	9.819	2634	2637	2641	rBV	294	252	0.01%	0.002%
73	9.883	2654	2657	2659	rBV2	190	141	0.01%	0.001%
74	9.912	2663	2666	2668	rVB	201	104	0.01%	0.001%
75	9.960	2677	2681	2686	rBV	244	304	0.02%	0.003%
76	10.102	2721	2725	2728	rBV2	144	119	0.01%	0.001%

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77	10.208	2754	2758	2761	rBV	224	170	0.01%	0.001%
78	10.291	2781	2784	2790	rVB2	387	359	0.02%	0.003%
79	10.533	2856	2859	2862	rBV	281	225	0.01%	0.002%
80	10.700	2909	2911	2916	rVB	249	118	0.01%	0.001%
81	10.758	2916	2929	2952	rBV	586997	946404	54.55%	8.096%
82	10.963	2990	2993	2996	rBV2	234	148	0.01%	0.001%
83	10.980	2996	2998	3000	rBV	190	124	0.01%	0.001%
84	11.118	3038	3041	3043	rBV	356	164	0.01%	0.001%
85	11.282	3090	3092	3099	rVB	293	243	0.01%	0.002%
86	11.452	3141	3145	3148	rBV	186	179	0.01%	0.002%
87	11.812	3245	3257	3273	rBV	439215	679759	39.18%	5.815%
88	11.973	3303	3307	3311	rBV2	183	169	0.01%	0.001%
89	11.996	3312	3314	3316	rVB	244	102	0.01%	0.001%
90	12.095	3342	3345	3349	rBV	322	273	0.02%	0.002%
91	12.195	3362	3376	3402	rBV	688494	1080437	62.27%	9.242%
92	12.401	3437	3440	3441	rBV	372	139	0.01%	0.001%
93	12.455	3453	3457	3464	rBV2	343	499	0.03%	0.004%
94	12.491	3465	3468	3471	rBV	302	272	0.02%	0.002%
95	12.639	3512	3514	3518	rBV	286	197	0.01%	0.002%
96	13.008	3626	3629	3637	rVB2	295	365	0.02%	0.003%
97	13.044	3637	3640	3643	rBV2	253	226	0.01%	0.002%
98	13.243	3698	3702	3704	rBV	469	295	0.02%	0.003%
99	13.481	3774	3776	3778	rBV	293	153	0.01%	0.001%
100	14.108	3969	3971	3973	rBV2	315	152	0.01%	0.001%

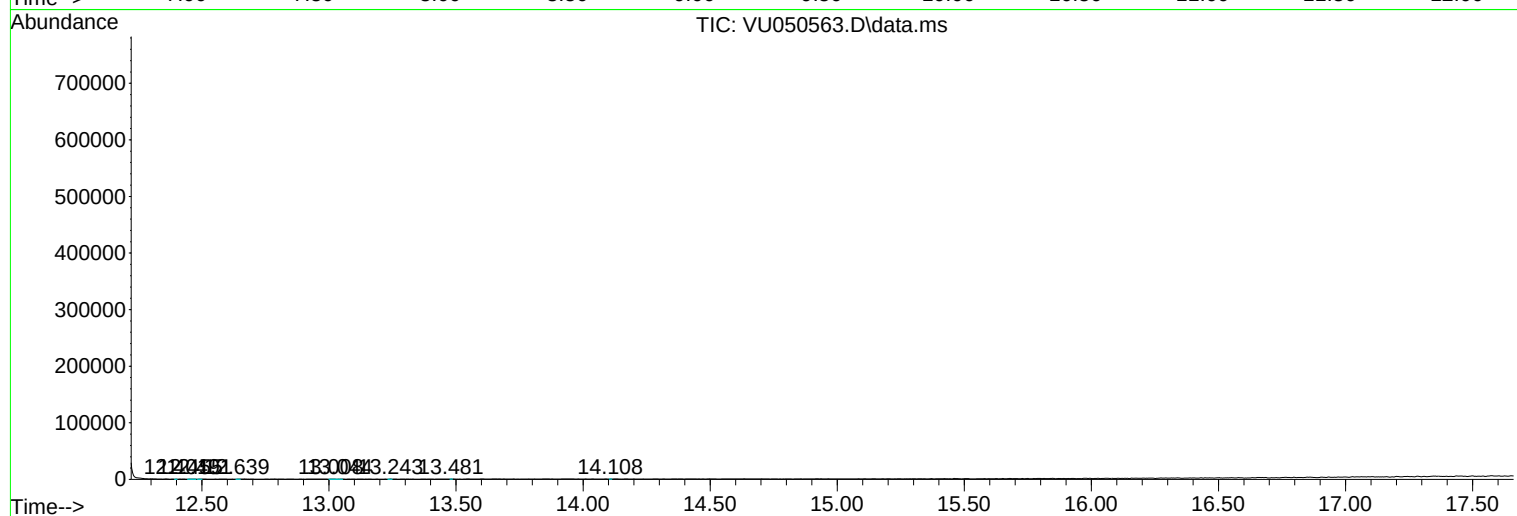
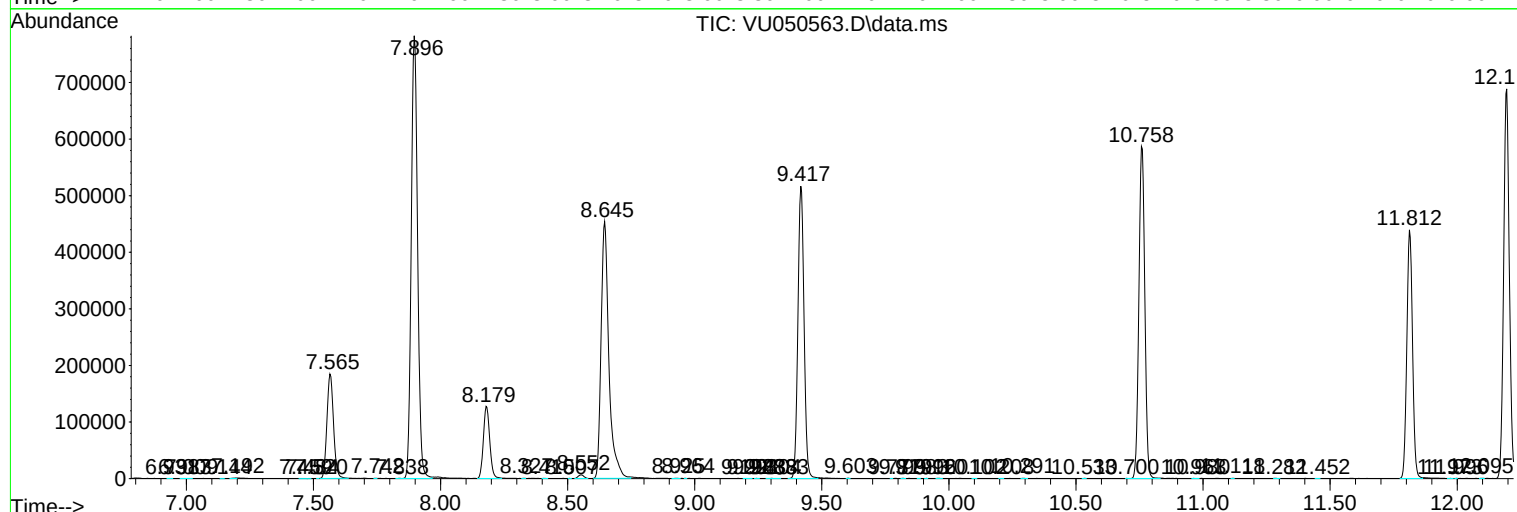
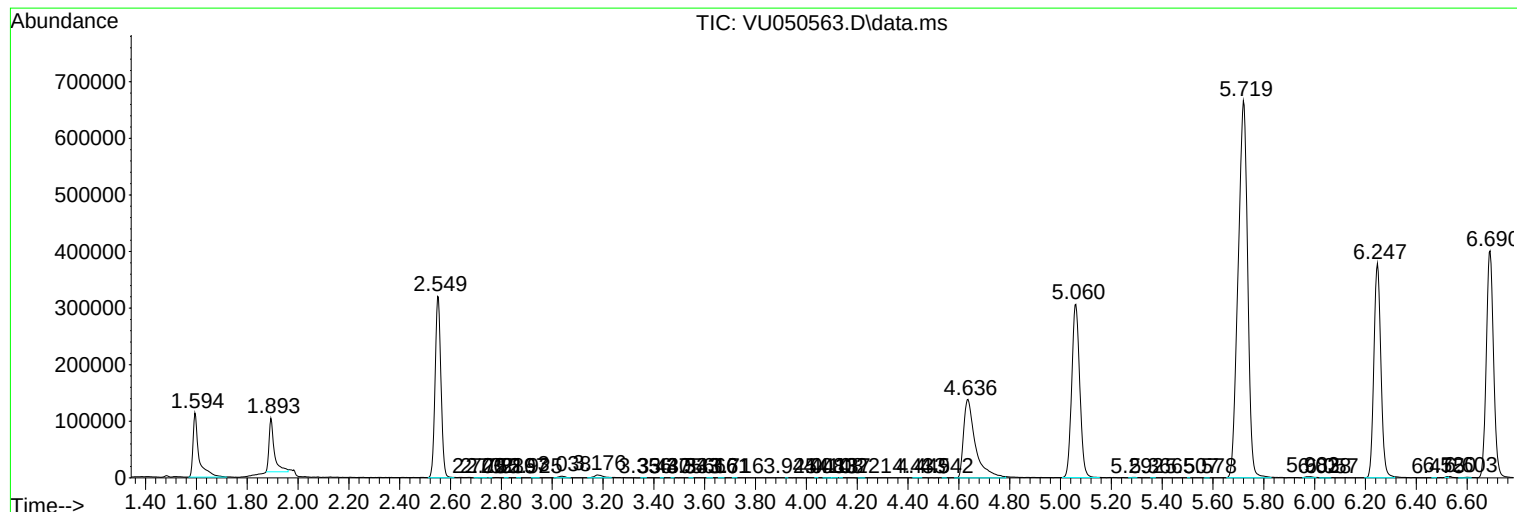
Sum of corrected areas: 11689904

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
Quant Title : VOC Analysis

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



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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