

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083122\
 Data File : VU050548.D
 Acq On : 31 Aug 2022 14:43
 Operator : SY/MD
 Sample : VU0831MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK174

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: VU050548.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	106	rBV	175351	225807	14.19%	2.140%
2	1.903	166	175	195	rVB	154056	211993	13.32%	2.009%
3	2.562	366	380	397	rBV	315927	507860	31.91%	4.813%
4	2.742	432	436	440	rBV3	409	335	0.02%	0.003%
5	2.790	440	451	459	rVB4	1413	2479	0.16%	0.023%
6	2.906	484	487	490	rVB	289	185	0.01%	0.002%
7	3.041	521	529	541	rVV4	2693	4551	0.29%	0.043%
8	3.096	542	546	549	rVB3	262	200	0.01%	0.002%
9	3.179	563	572	589	rBV3	2740	6424	0.40%	0.061%
10	3.266	595	599	605	rVB3	307	269	0.02%	0.003%
11	3.346	615	624	628	rBV5	1100	1315	0.08%	0.012%
12	3.475	660	664	666	rBV2	283	209	0.01%	0.002%
13	3.607	699	705	708	rBV2	304	313	0.02%	0.003%
14	3.758	749	752	756	rBV3	241	208	0.01%	0.002%
15	3.858	778	783	786	rBV2	366	357	0.02%	0.003%
16	4.356	932	938	942	rBV2	216	255	0.02%	0.002%
17	4.488	976	979	982	rBV2	286	212	0.01%	0.002%
18	4.626	1009	1022	1071	rBV	142297	411920	25.88%	3.904%
19	4.990	1133	1135	1142	rVB2	430	377	0.02%	0.004%
20	5.063	1142	1158	1183	rBV	284252	627640	39.43%	5.948%
21	5.272	1221	1223	1224	rBV	392	194	0.01%	0.002%
22	5.375	1252	1255	1259	rVV4	531	578	0.04%	0.005%
23	5.514	1294	1298	1300	rBV3	612	436	0.03%	0.004%
24	5.723	1342	1363	1386	rBV2	591165	1591731	100.00%	15.085%
25	5.883	1412	1413	1418	rVB3	319	174	0.01%	0.002%
26	5.983	1441	1444	1446	rVB3	355	196	0.01%	0.002%
27	6.031	1456	1459	1462	rBV2	432	363	0.02%	0.003%
28	6.247	1512	1526	1553	rBV	442803	848361	53.30%	8.040%
29	6.523	1608	1612	1613	rBV2	1041	662	0.04%	0.006%
30	6.591	1631	1633	1637	rVB2	261	186	0.01%	0.002%
31	6.690	1648	1664	1684	rBV	369981	726197	45.62%	6.882%
32	6.896	1724	1728	1732	rBV3	333	278	0.02%	0.003%
33	7.105	1786	1793	1796	rBV	585	689	0.04%	0.007%
34	7.189	1815	1819	1821	rBV2	492	404	0.03%	0.004%
35	7.282	1844	1848	1851	rBV	251	233	0.01%	0.002%
36	7.391	1878	1882	1886	rBV2	230	211	0.01%	0.002%

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

37	7.520	1917	1922	1924	rBV2	308	297	0.02%	0.003%
38	7.565	1924	1936	1966	rVV	167974	299958	18.84%	2.843%
39	7.800	2000	2009	2015	rBV3	1728	2540	0.16%	0.024%
40	7.899	2026	2040	2060	rBV	669683	1169059	73.45%	11.079%
41	8.179	2115	2127	2150	rBV	113669	197918	12.43%	1.876%
42	8.333	2172	2175	2180	rVB3	282	254	0.02%	0.002%
43	8.372	2184	2187	2190	rBV2	229	196	0.01%	0.002%
44	8.462	2213	2215	2218	rBV	415	271	0.02%	0.003%
45	8.501	2222	2227	2230	rVB2	386	270	0.02%	0.003%
46	8.562	2239	2246	2250	rVB2	1188	1378	0.09%	0.013%
47	8.636	2257	2269	2307	rBV4	317618	811676	50.99%	7.692%
48	8.841	2330	2333	2334	rBV	358	224	0.01%	0.002%
49	8.893	2346	2349	2350	rBV	332	181	0.01%	0.002%
50	8.922	2355	2358	2360	rBV4	649	487	0.03%	0.005%
51	9.140	2423	2426	2428	rBV	371	231	0.01%	0.002%
52	9.234	2449	2455	2458	rBV2	200	227	0.01%	0.002%
53	9.250	2458	2460	2464	rVB2	292	180	0.01%	0.002%
54	9.272	2464	2467	2470	rBV	369	268	0.02%	0.003%
55	9.417	2499	2512	2547	rBV	606680	1023472	64.30%	9.700%
56	9.693	2592	2598	2600	rBV3	658	669	0.04%	0.006%
57	9.902	2659	2663	2666	rBV2	445	442	0.03%	0.004%
58	10.105	2719	2726	2741	rBV7	1439	3196	0.20%	0.030%
59	10.166	2742	2745	2748	rVB	259	178	0.01%	0.002%
60	10.266	2773	2776	2778	rBV	252	201	0.01%	0.002%
61	10.330	2792	2796	2799	rBV	324	317	0.02%	0.003%
62	10.488	2836	2845	2852	rVV3	1096	1806	0.11%	0.017%
63	10.636	2884	2891	2901	rVB4	2110	3027	0.19%	0.029%
64	10.755	2915	2928	2962	rBV	409344	689863	43.34%	6.538%
65	10.870	2962	2964	2970	rVB2	458	338	0.02%	0.003%
66	10.960	2989	2992	2994	rBV2	297	218	0.01%	0.002%
67	11.012	3003	3008	3011	rBV2	240	301	0.02%	0.003%
68	11.037	3012	3016	3018	rVV2	292	261	0.02%	0.002%
69	11.054	3018	3021	3024	rVV	225	209	0.01%	0.002%
70	11.092	3026	3033	3036	rVV2	765	1061	0.07%	0.010%
71	11.308	3096	3100	3104	rBV2	251	270	0.02%	0.003%
72	11.388	3122	3125	3129	rVB2	264	229	0.01%	0.002%
73	11.430	3135	3138	3143	rVB2	313	276	0.02%	0.003%
74	11.468	3144	3150	3152	rBV	885	897	0.06%	0.009%
75	11.677	3210	3215	3218	rBV2	290	218	0.01%	0.002%
76	11.700	3218	3222	3224	rBV2	243	215	0.01%	0.002%

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 Title : VOC Analysis

77	11.745	3230	3236	3245	rVB4	1514	2215	0.14%	0.021%
78	11.812	3245	3257	3281	rBV	318629	510379	32.06%	4.837%
79	11.976	3305	3308	3312	rBV2	515	417	0.03%	0.004%
80	12.005	3312	3317	3320	rVB	316	330	0.02%	0.003%
81	12.037	3320	3327	3331	rBV3	341	449	0.03%	0.004%
82	12.195	3363	3376	3403	rBV	360385	605554	38.04%	5.739%
83	12.497	3468	3470	3473	rVB2	411	244	0.02%	0.002%
84	12.517	3473	3476	3480	rBV	283	223	0.01%	0.002%
85	12.536	3480	3482	3488	rVV2	313	348	0.02%	0.003%
86	12.626	3504	3510	3511	rBV	267	196	0.01%	0.002%
87	12.828	3569	3573	3576	rBV2	245	242	0.02%	0.002%
88	12.944	3605	3609	3612	rBV2	248	216	0.01%	0.002%
89	13.140	3668	3670	3673	rBV2	239	189	0.01%	0.002%
90	13.227	3690	3697	3708	rVB6	2111	3025	0.19%	0.029%
91	13.314	3720	3724	3728	rVB2	353	321	0.02%	0.003%
92	13.468	3769	3772	3776	rVB2	398	293	0.02%	0.003%
93	13.500	3778	3782	3785	rBV	394	280	0.02%	0.003%
94	13.610	3813	3816	3820	rBV3	267	250	0.02%	0.002%
95	13.725	3850	3852	3855	rBV	443	281	0.02%	0.003%
96	13.848	3881	3890	3899	rBV6	4273	7154	0.45%	0.068%
97	14.092	3958	3966	3986	rVB	10738	19124	1.20%	0.181%
98	14.333	4032	4041	4053	rBV4	6554	11387	0.72%	0.108%
99	15.098	4276	4279	4281	rBV	613	424	0.03%	0.004%
100	15.269	4329	4332	4339	rBV3	965	999	0.06%	0.009%

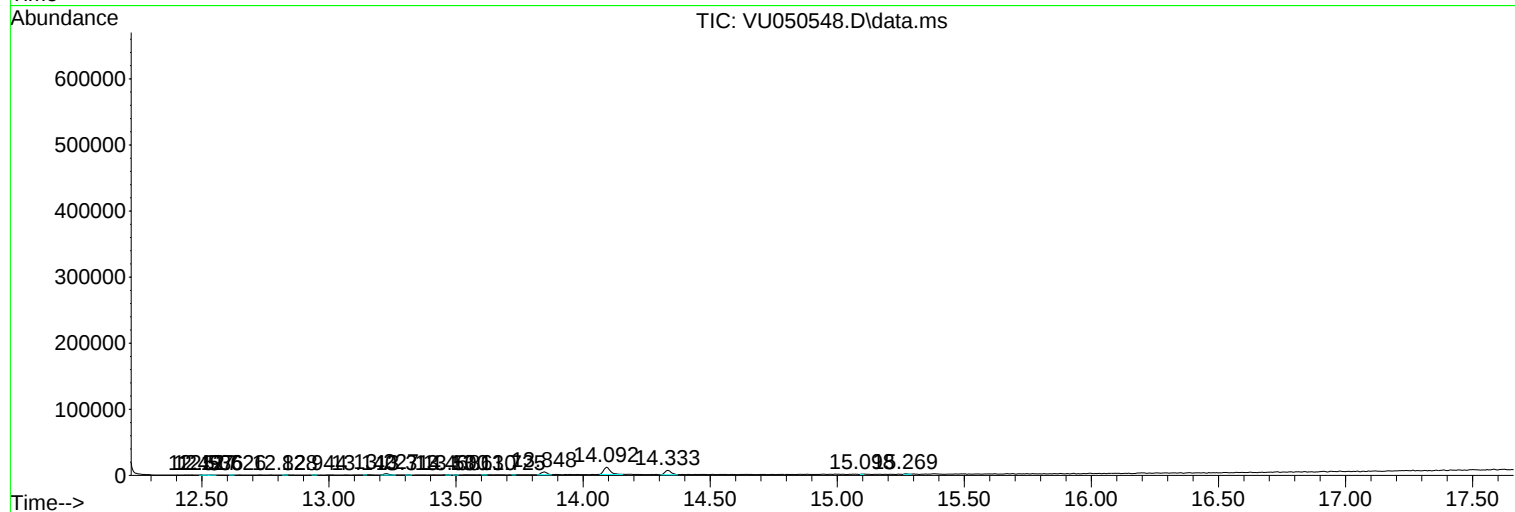
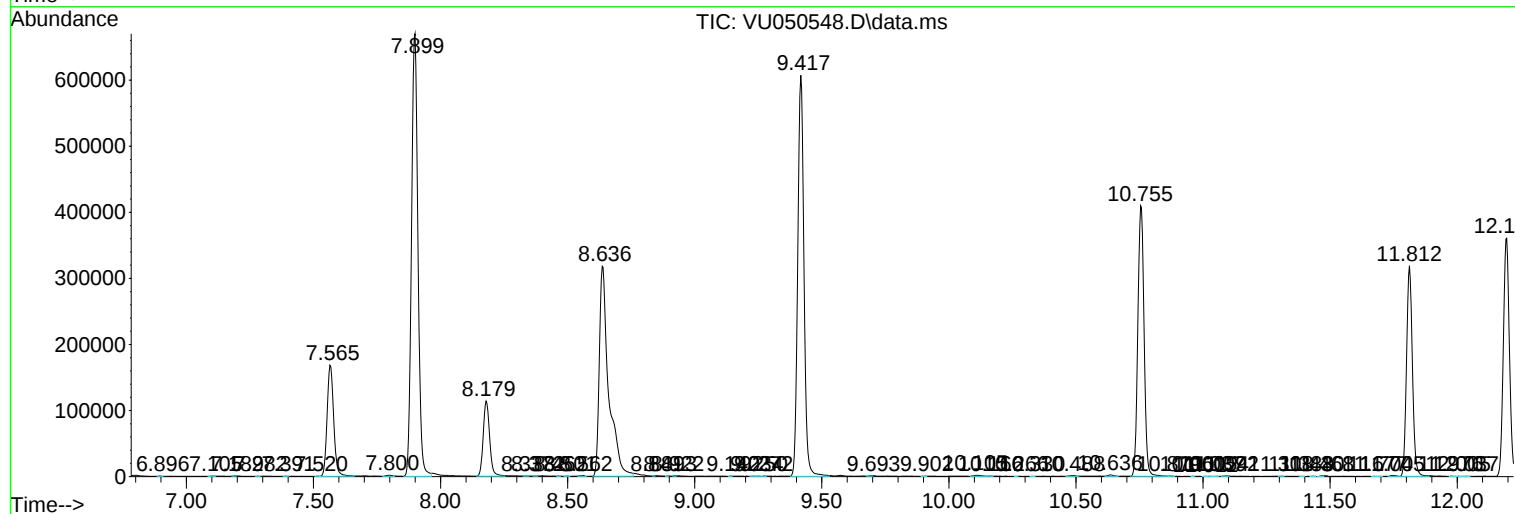
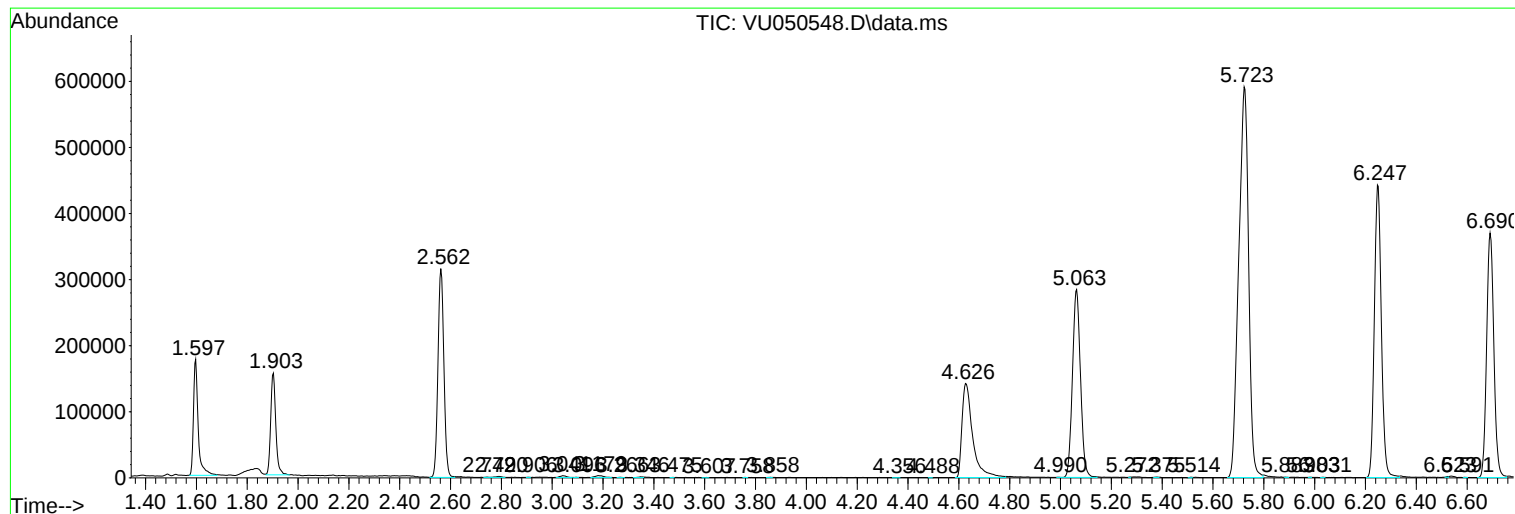
Sum of corrected areas: 10551621

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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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Instrument :
MSVOA_U
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VBLK174

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

No Library Search Compounds Detected

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
