

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU083122\  
 Data File : VU050557.D  
 Acq On : 31 Aug 2022 18:31  
 Operator : SY/MD  
 Sample : N4363-15ME  
 Misc : 5.51g/5.0mL/100uL/5.0mL/MSVOA\_U/MEOH  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 DBVW9ME

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: VU050557.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	40	44	49	rBV4	3324	3560	0.14%	0.023%
2	1.594	71	79	89	rBV	152182	219195	8.68%	1.445%
3	1.890	166	171	180	rBV	58095	79903	3.17%	0.527%
4	2.530	357	370	400	rVB	480939	787498	31.20%	5.193%
5	2.755	436	440	441	rBV	424	327	0.01%	0.002%
6	3.031	511	526	540	rBV3	7565	16050	0.64%	0.106%
7	3.108	547	550	554	rVB2	675	563	0.02%	0.004%
8	3.179	554	572	594	rBV2	14196	41938	1.66%	0.277%
9	3.423	645	648	653	rVB2	454	320	0.01%	0.002%
10	3.665	718	723	734	rVB6	972	1841	0.07%	0.012%
11	3.777	755	758	762	rVB	356	221	0.01%	0.001%
12	3.845	776	779	782	rBV	259	212	0.01%	0.001%
13	3.874	785	788	792	rVV	381	276	0.01%	0.002%
14	4.147	869	873	876	rBV	350	257	0.01%	0.002%
15	4.485	975	978	986	rBV2	175	217	0.01%	0.001%
16	4.642	1011	1027	1104	rBV	173727	668858	26.50%	4.411%
17	4.976	1129	1131	1135	rBV	327	211	0.01%	0.001%
18	5.060	1139	1157	1185	rVV2	414186	967088	38.31%	6.377%
19	5.285	1220	1227	1228	rBV4	1174	1212	0.05%	0.008%
20	5.359	1247	1250	1253	rBV2	823	709	0.03%	0.005%
21	5.716	1340	1361	1394	rBV2	998368	2524218	100.00%	16.646%
22	5.980	1432	1443	1463	rBV2	11009	28079	1.11%	0.185%
23	6.102	1478	1481	1483	rBV2	362	291	0.01%	0.002%
24	6.247	1510	1526	1553	rBV	526153	1054148	41.76%	6.951%
25	6.404	1573	1575	1580	rVB3	391	267	0.01%	0.002%
26	6.526	1604	1613	1614	rBV5	5731	6653	0.26%	0.044%
27	6.603	1627	1637	1648	rBV3	5121	11212	0.44%	0.074%
28	6.690	1649	1664	1690	rVV	559629	1152103	45.64%	7.597%
29	7.224	1815	1830	1848	rBV8	4861	13852	0.55%	0.091%
30	7.314	1850	1858	1859	rBV3	856	809	0.03%	0.005%
31	7.507	1917	1918	1924	rBV	292	249	0.01%	0.002%
32	7.568	1924	1937	1961	rBV	246063	476034	18.86%	3.139%
33	7.703	1977	1979	1989	rVB3	860	943	0.04%	0.006%
34	7.838	2019	2021	2025	rVB2	441	233	0.01%	0.002%
35	7.899	2025	2040	2062	rBV	1064288	1946188	77.10%	12.834%
36	7.992	2063	2069	2089	rVB3	7442	18598	0.74%	0.123%

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 DBVW9ME

Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
 Start Thrs : 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 0 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

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

37	8.182	2116	2128	2150	rBV	152820	303746	12.03%	2.003%
38	8.304	2164	2166	2168	rBV2	350	216	0.01%	0.001%
39	8.317	2168	2170	2173	rVV3	594	355	0.01%	0.002%
40	8.356	2174	2182	2186	rVV8	1140	1787	0.07%	0.012%
41	8.375	2186	2188	2191	rVB3	487	230	0.01%	0.002%
42	8.552	2234	2243	2253	rBV2	10931	18394	0.73%	0.121%
43	8.661	2258	2277	2311	rBV3	488583	1296363	51.36%	8.549%
44	9.201	2443	2445	2451	rVB2	334	245	0.01%	0.002%
45	9.420	2499	2513	2544	rBV	624304	1158419	45.89%	7.639%
46	9.574	2557	2561	2563	rBV3	379	355	0.01%	0.002%
47	9.616	2569	2574	2577	rBV3	507	405	0.02%	0.003%
48	10.079	2715	2718	2721	rBV2	366	274	0.01%	0.002%
49	10.407	2818	2820	2827	rVB	343	285	0.01%	0.002%
50	10.539	2857	2861	2864	rBV2	294	252	0.01%	0.002%
51	10.574	2869	2872	2876	rBV2	206	215	0.01%	0.001%
52	10.764	2917	2931	2948	rBV	505333	841554	33.34%	5.549%
53	10.902	2970	2974	2978	rBV	338	217	0.01%	0.001%
54	10.983	2994	2999	3003	rBV2	217	262	0.01%	0.002%
55	11.063	3018	3024	3029	rBV2	328	391	0.02%	0.003%
56	11.095	3029	3034	3035	rBV	345	237	0.01%	0.002%
57	11.121	3035	3042	3046	rVV6	609	918	0.04%	0.006%
58	11.317	3095	3103	3104	rBV	260	249	0.01%	0.002%
59	11.365	3114	3118	3121	rVB2	388	253	0.01%	0.002%
60	11.385	3121	3124	3132	rBV2	315	291	0.01%	0.002%
61	11.497	3156	3159	3166	rBV2	252	298	0.01%	0.002%
62	11.590	3183	3188	3191	rBV2	382	282	0.01%	0.002%
63	11.635	3198	3202	3206	rVB2	244	233	0.01%	0.002%
64	11.815	3245	3258	3274	rBV	369435	589670	23.36%	3.888%
65	11.954	3298	3301	3305	rVB3	397	341	0.01%	0.002%
66	12.092	3340	3344	3349	rVB2	291	286	0.01%	0.002%
67	12.143	3356	3360	3363	rBV	337	288	0.01%	0.002%
68	12.195	3363	3376	3393	rBV	570151	912426	36.15%	6.017%
69	12.323	3413	3416	3418	rBV	371	206	0.01%	0.001%
70	12.365	3426	3429	3435	rVB3	326	349	0.01%	0.002%
71	12.420	3443	3446	3450	rVB	361	276	0.01%	0.002%
72	12.545	3482	3485	3488	rBV	280	222	0.01%	0.001%
73	12.584	3493	3497	3500	rBV	278	258	0.01%	0.002%
74	12.635	3510	3513	3520	rVB2	231	219	0.01%	0.001%
75	12.677	3524	3526	3531	rVB2	281	209	0.01%	0.001%
76	12.748	3539	3548	3550	rBV2	324	289	0.01%	0.002%

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 Title : VOC Analysis

77	12.848	3576	3579	3584	rVV2	224	221	0.01%	0.001%
78	12.999	3623	3626	3630	rVB	310	214	0.01%	0.001%
79	13.076	3648	3650	3657	rVB2	359	311	0.01%	0.002%
80	13.147	3667	3672	3673	rBV	275	232	0.01%	0.002%
81	13.217	3689	3694	3697	rVB3	363	330	0.01%	0.002%
82	13.240	3697	3701	3706	rVB2	246	224	0.01%	0.001%
83	13.278	3708	3713	3716	rVB2	341	267	0.01%	0.002%
84	13.323	3723	3727	3729	rBV2	359	280	0.01%	0.002%
85	13.500	3777	3782	3786	rVB2	283	333	0.01%	0.002%
86	13.561	3797	3801	3805	rBV2	265	285	0.01%	0.002%
87	13.651	3824	3829	3832	rVB3	360	315	0.01%	0.002%
88	13.761	3858	3863	3868	rBV3	344	465	0.02%	0.003%
89	13.889	3896	3903	3907	rBV2	410	507	0.02%	0.003%
90	13.957	3921	3924	3930	rVB2	464	492	0.02%	0.003%
91	14.089	3960	3965	3967	rBV2	475	523	0.02%	0.003%
92	14.208	3996	4002	4006	rBV3	385	503	0.02%	0.003%
93	14.404	4060	4063	4067	rBV2	265	292	0.01%	0.002%
94	14.465	4078	4082	4084	rBV2	400	331	0.01%	0.002%
95	14.497	4089	4092	4096	rVB3	294	219	0.01%	0.001%
96	14.655	4137	4141	4147	rBV4	461	597	0.02%	0.004%
97	14.700	4153	4155	4161	rVB2	420	313	0.01%	0.002%
98	15.494	4398	4402	4405	rBV4	364	333	0.01%	0.002%
99	15.587	4429	4431	4433	rBV2	425	300	0.01%	0.002%
100	15.693	4461	4464	4467	rVB2	668	524	0.02%	0.003%

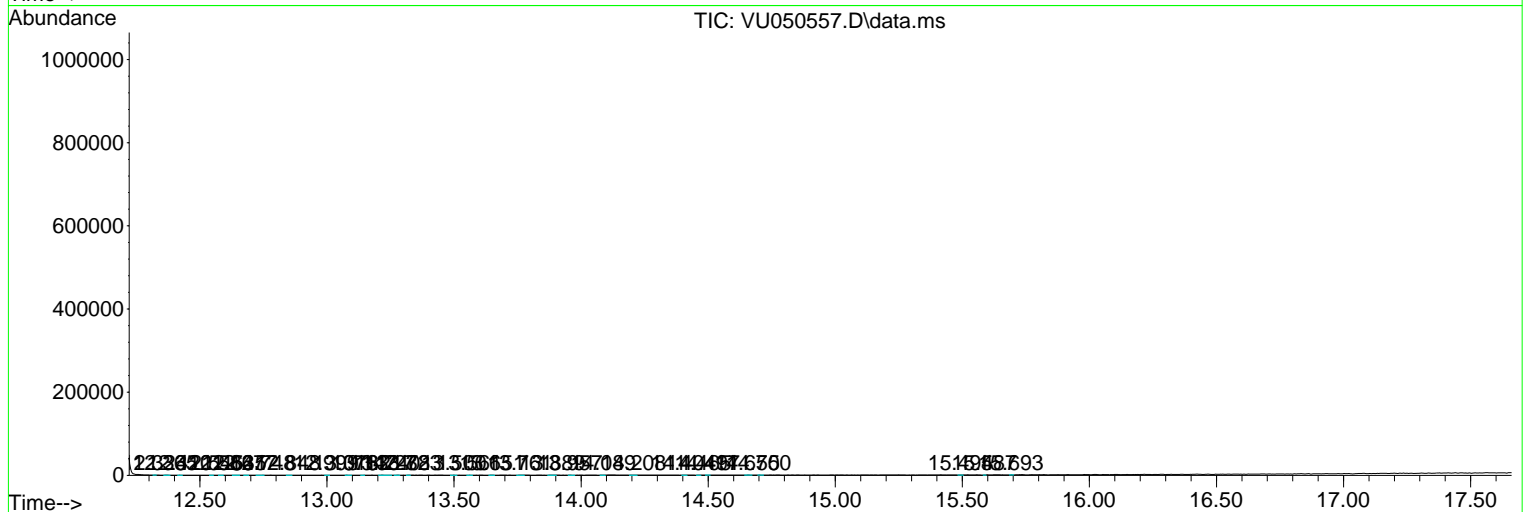
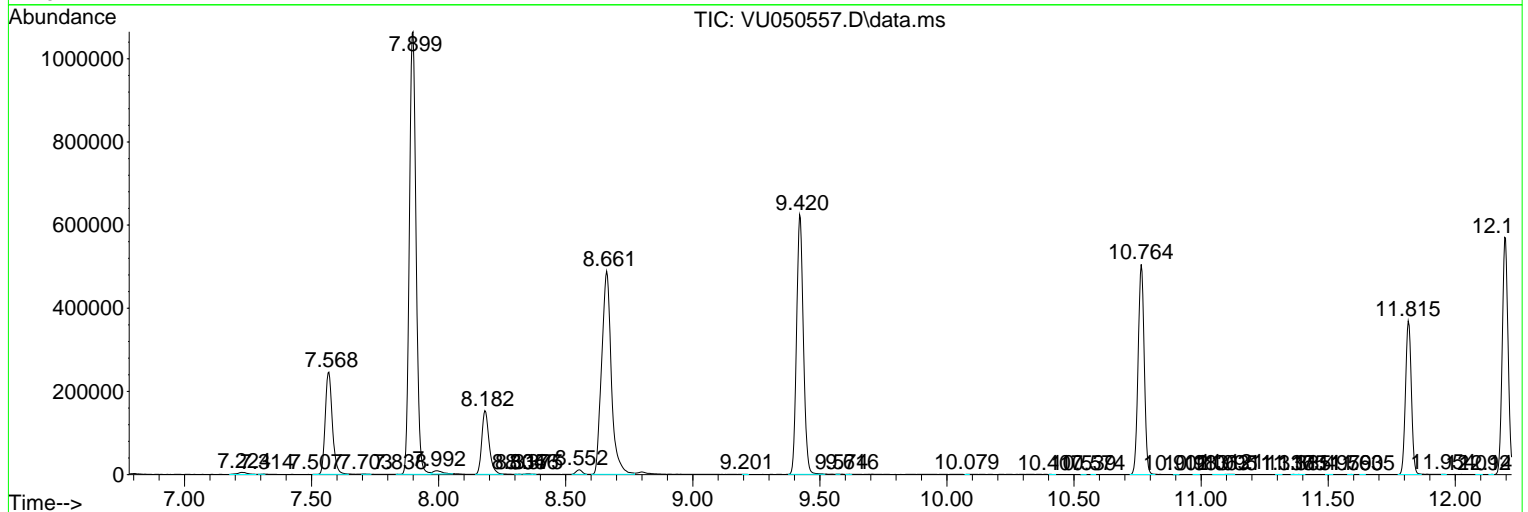
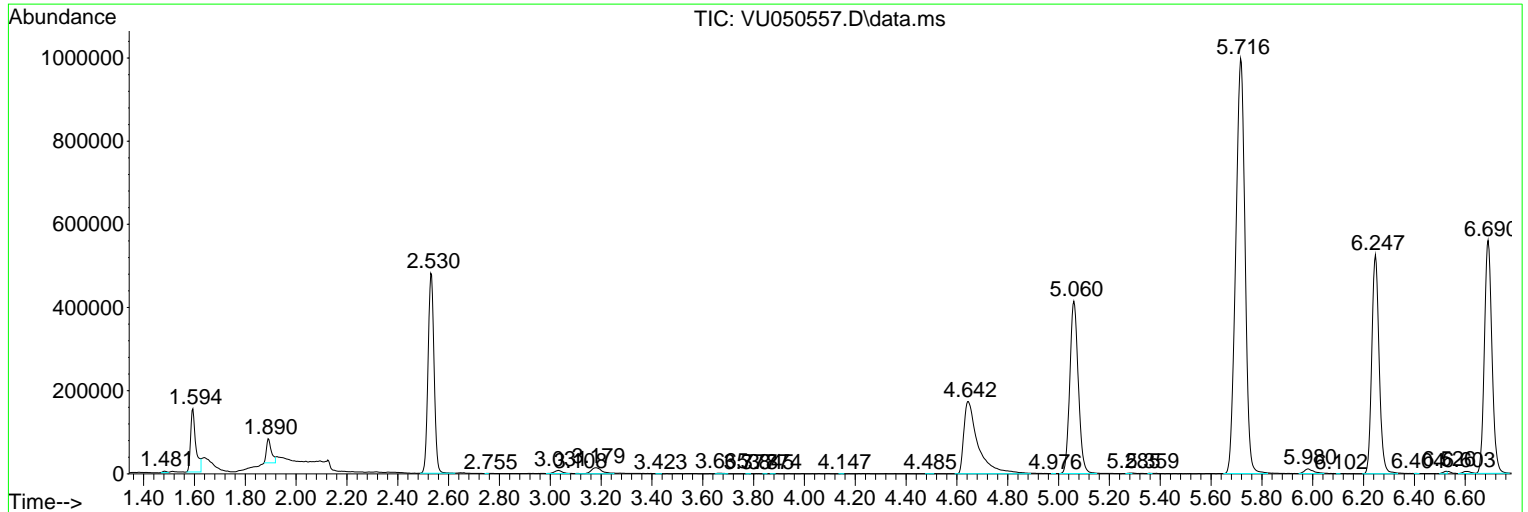
Sum of corrected areas: 15164509

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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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU083122\  
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Instrument :  
MSVOA\_U  
ClientSampleId :  
DBVW9ME

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

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