

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051822\
 Data File : VU048607.D
 Acq On : 18 May 2022 11:50
 Operator : SY/MD
 Sample : VU0518MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK130

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\SFAMULM051622WMA.M

Title : VOC Analysis

Signal : TIC: VU048607.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	99	rVB	77346	88982	10.39%	1.279%
2	1.912	170	178	197	rVB	65896	85942	10.04%	1.235%
3	2.282	291	293	299	rBV2	176	156	0.02%	0.002%
4	2.356	312	316	319	rBV2	249	198	0.02%	0.003%
5	2.568	370	382	398	rBV	174476	285880	33.38%	4.109%
6	2.735	428	434	437	rBV	265	306	0.04%	0.004%
7	2.790	446	451	454	rBV2	363	364	0.04%	0.005%
8	2.916	488	490	495	rBB	177	161	0.02%	0.002%
9	3.044	523	530	537	rBV2	1196	1696	0.20%	0.024%
10	3.118	550	553	556	rBB	290	201	0.02%	0.003%
11	3.147	559	562	565	rBV	159	147	0.02%	0.002%
12	3.272	597	601	604	rBB	246	192	0.02%	0.003%
13	3.694	727	732	736	rBB	206	229	0.03%	0.003%
14	4.086	850	854	856	rBB	212	159	0.02%	0.002%
15	4.353	933	937	939	rBB	222	157	0.02%	0.002%
16	4.430	957	961	964	rBB	204	148	0.02%	0.002%
17	4.623	1007	1021	1051	rBV	82672	208571	24.36%	2.997%
18	4.890	1101	1104	1107	rVB2	316	263	0.03%	0.004%
19	4.919	1108	1113	1116	rBB2	321	256	0.03%	0.004%
20	5.067	1141	1159	1181	rBV	166651	369604	43.16%	5.312%
21	5.157	1186	1187	1191	rVB2	267	146	0.02%	0.002%
22	5.726	1342	1364	1383	rBV2	314464	856324	100.00%	12.307%
23	5.890	1413	1415	1419	rVB2	510	329	0.04%	0.005%
24	5.931	1425	1428	1429	rBV	284	165	0.02%	0.002%
25	6.044	1461	1463	1467	rBV	294	187	0.02%	0.003%
26	6.115	1483	1485	1488	rBB	291	157	0.02%	0.002%
27	6.144	1491	1494	1496	rBB	250	144	0.02%	0.002%
28	6.250	1513	1527	1551	rBV	273008	513730	59.99%	7.383%
29	6.411	1572	1577	1580	rBV	272	205	0.02%	0.003%
30	6.475	1594	1597	1600	rVV	196	163	0.02%	0.002%
31	6.533	1605	1615	1624	rVV2	3826	7370	0.86%	0.106%
32	6.607	1633	1638	1642	rBB	292	309	0.04%	0.004%
33	6.693	1651	1665	1686	rBV	190624	375054	43.80%	5.390%
34	6.809	1697	1701	1705	rBV2	679	553	0.06%	0.008%
35	7.050	1772	1776	1778	rBB2	319	254	0.03%	0.004%
36	7.185	1812	1818	1821	rBV3	1063	1040	0.12%	0.015%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
 Title : VOC Analysis

37	7.211	1825	1826	1830	rVB	274	179	0.02%	0.003%
38	7.243	1834	1836	1840	rVB	221	152	0.02%	0.002%
39	7.275	1841	1846	1849	rBB	281	206	0.02%	0.003%
40	7.311	1852	1857	1861	rBB	147	190	0.02%	0.003%
41	7.568	1925	1937	1957	rBV	114365	204054	23.83%	2.933%
42	7.693	1968	1976	1983	rVB5	1245	1937	0.23%	0.028%
43	7.774	1998	2001	2002	rBV	326	187	0.02%	0.003%
44	7.787	2003	2005	2016	rVB4	571	751	0.09%	0.011%
45	7.899	2025	2040	2055	rBV	405599	690801	80.67%	9.928%
46	8.118	2105	2108	2113	rBB	193	211	0.02%	0.003%
47	8.179	2116	2127	2145	rBV	86190	148064	17.29%	2.128%
48	8.427	2199	2204	2207	rBV	259	315	0.04%	0.005%
49	8.481	2219	2221	2226	rVB2	345	319	0.04%	0.005%
50	8.555	2242	2244	2250	rBB	335	251	0.03%	0.004%
51	8.636	2256	2269	2308	rBV2	261834	491375	57.38%	7.062%
52	9.057	2397	2400	2402	rBV	184	151	0.02%	0.002%
53	9.066	2402	2403	2408	rVB2	165	152	0.02%	0.002%
54	9.163	2431	2433	2436	rVB2	425	233	0.03%	0.003%
55	9.256	2458	2462	2464	rBV	168	160	0.02%	0.002%
56	9.285	2468	2471	2473	rBV	171	146	0.02%	0.002%
57	9.417	2499	2512	2537	rBV	390022	657722	76.81%	9.452%
58	9.639	2578	2581	2583	rBV	305	231	0.03%	0.003%
59	9.693	2592	2598	2605	rBV2	961	1170	0.14%	0.017%
60	9.742	2611	2613	2616	rVB	298	186	0.02%	0.003%
61	9.771	2616	2622	2626	rBV2	292	377	0.04%	0.005%
62	9.832	2637	2641	2644	rBB	209	202	0.02%	0.003%
63	9.867	2644	2652	2657	rBV	188	391	0.05%	0.006%
64	10.070	2712	2715	2717	rBV	193	152	0.02%	0.002%
65	10.102	2721	2725	2728	rBV3	557	478	0.06%	0.007%
66	10.311	2786	2790	2793	rBV	240	250	0.03%	0.004%
67	10.401	2815	2818	2821	rBV	345	241	0.03%	0.003%
68	10.459	2832	2836	2841	rBV	278	297	0.03%	0.004%
69	10.488	2841	2845	2848	rVB2	595	393	0.05%	0.006%
70	10.600	2873	2880	2884	rBV	225	327	0.04%	0.005%
71	10.635	2885	2891	2897	rVV5	1379	1736	0.20%	0.025%
72	10.674	2897	2903	2909	rVV4	1230	1161	0.14%	0.017%
73	10.758	2916	2929	2948	rVB	296272	476888	55.69%	6.854%
74	10.867	2960	2963	2967	rVB	276	183	0.02%	0.003%
75	10.967	2988	2994	2999	rBB	217	325	0.04%	0.005%
76	10.999	3000	3004	3007	rBV	429	367	0.04%	0.005%

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77	11.176	3053	3059	3062	rBV	242	353	0.04%	0.005%
78	11.282	3088	3092	3093	rBV	247	145	0.02%	0.002%
79	11.414	3131	3133	3135	rBV	415	245	0.03%	0.004%
80	11.462	3142	3148	3149	rBV3	684	491	0.06%	0.007%
81	11.597	3186	3190	3196	rBV	239	326	0.04%	0.005%
82	11.693	3215	3220	3221	rBV	299	190	0.02%	0.003%
83	11.748	3232	3237	3243	rBV3	809	975	0.11%	0.014%
84	11.812	3244	3257	3275	rBV	456473	722862	84.41%	10.389%
85	11.944	3295	3298	3300	rVB2	355	202	0.02%	0.003%
86	12.195	3363	3376	3399	rBV	447420	728939	85.12%	10.476%
87	12.549	3483	3486	3488	rBV	217	154	0.02%	0.002%
88	12.767	3552	3554	3560	rVB2	324	208	0.02%	0.003%
89	12.819	3568	3570	3574	rBV	246	147	0.02%	0.002%
90	12.909	3594	3598	3601	rBV2	424	274	0.03%	0.004%
91	13.005	3626	3628	3631	rVV2	351	159	0.02%	0.002%
92	13.230	3691	3698	3705	rVB4	848	1137	0.13%	0.016%
93	13.844	3883	3889	3898	rVB4	2217	2686	0.31%	0.039%
94	13.883	3898	3901	3904	rVB	312	167	0.02%	0.002%
95	14.008	3938	3940	3943	rBV	293	161	0.02%	0.002%
96	14.092	3958	3966	3975	rBV2	7218	10976	1.28%	0.158%
97	14.272	4019	4022	4026	rBV2	409	462	0.05%	0.007%
98	14.336	4034	4042	4052	rVB6	2099	3463	0.40%	0.050%
99	14.664	4142	4144	4147	rVB	474	210	0.02%	0.003%
100	15.548	4417	4419	4425	rVB3	793	601	0.07%	0.009%

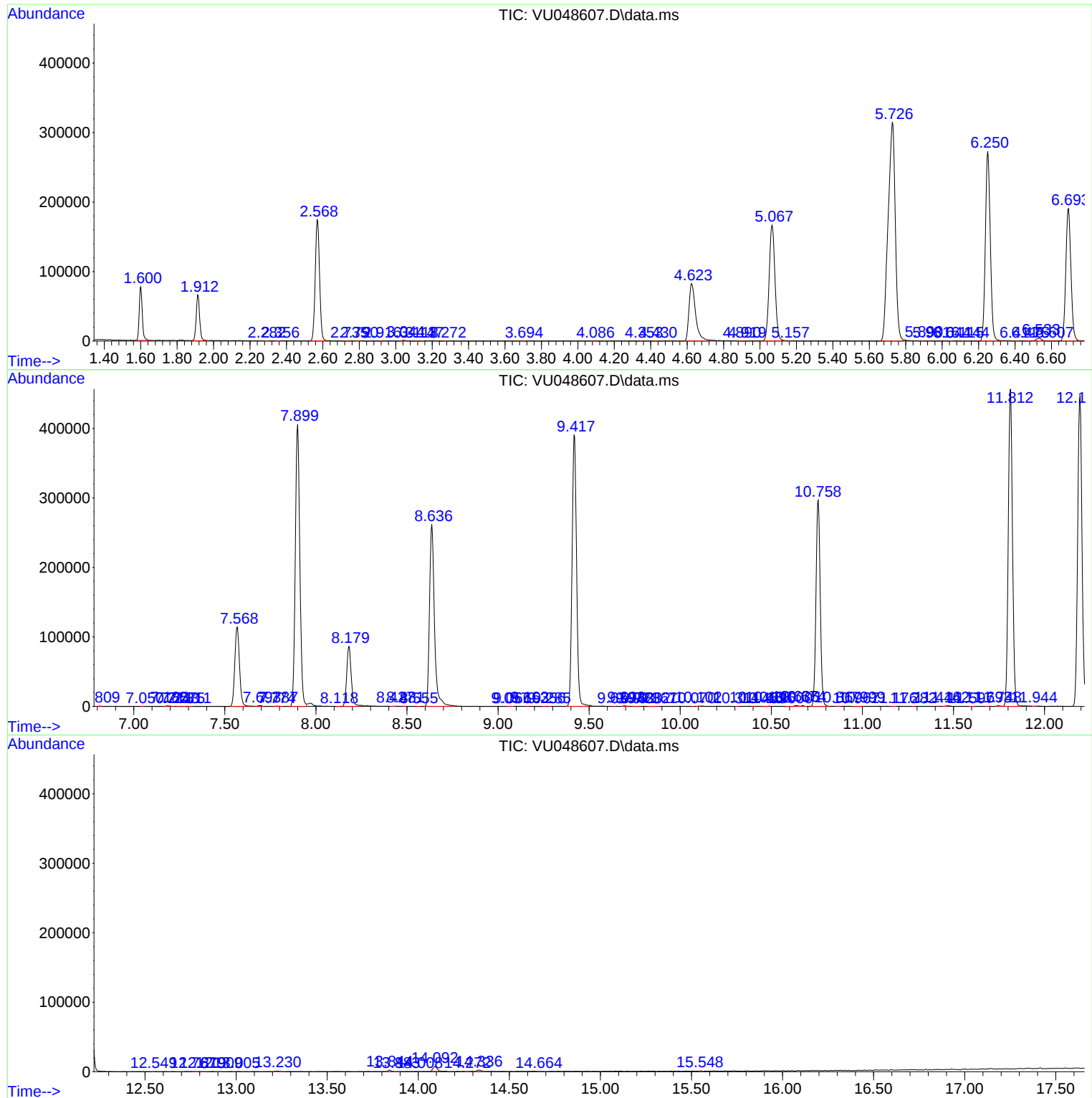
Sum of corrected areas: 6958186

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.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