

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051722\
 Data File : VU048599.D
 Acq On : 17 May 2022 12:39
 Operator : SY/MD
 Sample : VU0517WBL01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 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\SFAMULM051622WMA.M

Title : VOC Analysis

Signal : TIC: VU048599.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	103	rVB	84631	91677	10.95%	1.368%
2	1.912	170	178	192	rVB	63024	81243	9.70%	1.212%
3	2.366	317	319	321	rBV	357	151	0.02%	0.002%
4	2.568	371	382	399	rBV	173532	281866	33.67%	4.206%
5	2.800	447	454	462	rBB	692	963	0.12%	0.014%
6	2.906	485	487	490	rVB	294	153	0.02%	0.002%
7	2.954	499	502	506	rBB	288	255	0.03%	0.004%
8	2.986	509	512	516	rBB	147	151	0.02%	0.002%
9	3.044	525	530	532	rBV2	772	679	0.08%	0.010%
10	3.134	555	558	561	rBV	157	159	0.02%	0.002%
11	3.179	565	572	587	rVB	1305	2870	0.34%	0.043%
12	3.279	600	603	606	rBB	266	199	0.02%	0.003%
13	3.398	637	640	644	rBB	190	195	0.02%	0.003%
14	3.729	740	743	748	rBB	191	201	0.02%	0.003%
15	3.967	814	817	820	rBB	263	174	0.02%	0.003%
16	4.057	842	845	847	rVB	318	186	0.02%	0.003%
17	4.620	1007	1020	1063	rBV	88390	213510	25.50%	3.186%
18	4.845	1087	1090	1094	rVB2	303	246	0.03%	0.004%
19	4.887	1100	1103	1105	rVB	320	186	0.02%	0.003%
20	4.919	1110	1113	1118	rBV2	440	466	0.06%	0.007%
21	4.941	1118	1120	1122	rVB	335	171	0.02%	0.003%
22	5.063	1142	1158	1183	rBV	165380	362355	43.28%	5.407%
23	5.289	1225	1228	1229	rBV	335	181	0.02%	0.003%
24	5.726	1343	1364	1383	rBV2	300027	837266	100.00%	12.493%
25	5.893	1414	1416	1420	rBV	188	144	0.02%	0.002%
26	5.925	1423	1426	1428	rBV	301	201	0.02%	0.003%
27	5.951	1432	1434	1436	rBV	269	153	0.02%	0.002%
28	6.015	1449	1454	1457	rBB2	302	217	0.03%	0.003%
29	6.057	1462	1467	1470	rBB2	361	265	0.03%	0.004%
30	6.083	1471	1475	1478	rBV	236	232	0.03%	0.003%
31	6.250	1511	1527	1547	rBV2	263405	498557	59.55%	7.439%
32	6.530	1604	1614	1625	rBV5	4300	7628	0.91%	0.114%
33	6.639	1644	1648	1651	rBB	166	156	0.02%	0.002%
34	6.690	1651	1664	1684	rBV	188667	366020	43.72%	5.461%
35	6.780	1688	1692	1695	rBV	260	243	0.03%	0.004%
36	6.813	1700	1702	1707	rVB3	510	328	0.04%	0.005%

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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

37	7.009	1758	1763	1766	rBB	186	219	0.03%	0.003%
38	7.099	1787	1791	1794	rBB	221	204	0.02%	0.003%
39	7.173	1812	1814	1815	rBV	468	234	0.03%	0.003%
40	7.227	1826	1831	1834	rBV	203	236	0.03%	0.004%
41	7.459	1899	1903	1908	rBB2	287	307	0.04%	0.005%
42	7.517	1918	1921	1924	rBV	176	176	0.02%	0.003%
43	7.565	1924	1936	1955	rBV	107500	192458	22.99%	2.872%
44	7.684	1969	1973	1977	rBV3	839	870	0.10%	0.013%
45	7.758	1994	1996	2000	rBB	217	151	0.02%	0.002%
46	7.832	2016	2019	2022	rBV	229	206	0.02%	0.003%
47	7.899	2026	2040	2058	rBV	387385	663461	79.24%	9.899%
48	8.179	2114	2127	2143	rBV2	84920	142652	17.04%	2.128%
49	8.382	2185	2190	2195	rBV2	258	322	0.04%	0.005%
50	8.411	2196	2199	2202	rVB2	335	223	0.03%	0.003%
51	8.459	2210	2214	2219	rBV2	399	458	0.05%	0.007%
52	8.558	2242	2245	2247	rBV	197	164	0.02%	0.002%
53	8.632	2255	2268	2295	rBV	246639	466073	55.67%	6.954%
54	8.851	2334	2336	2338	rVB	373	165	0.02%	0.002%
55	8.886	2341	2347	2350	rBB	238	265	0.03%	0.004%
56	9.025	2387	2390	2394	rVB	198	147	0.02%	0.002%
57	9.066	2398	2403	2408	rBV	307	362	0.04%	0.005%
58	9.121	2417	2420	2424	rVB	236	208	0.02%	0.003%
59	9.198	2441	2444	2447	rBV	192	174	0.02%	0.003%
60	9.269	2463	2466	2468	rBV	205	159	0.02%	0.002%
61	9.356	2488	2493	2496	rBB	299	247	0.03%	0.004%
62	9.417	2500	2512	2538	rBV	381688	633316	75.64%	9.450%
63	9.562	2552	2557	2559	rBV	505	441	0.05%	0.007%
64	9.600	2566	2569	2571	rBV	288	220	0.03%	0.003%
65	9.632	2576	2579	2581	rBV	213	170	0.02%	0.003%
66	9.690	2593	2597	2605	rVV3	517	781	0.09%	0.012%
67	9.735	2609	2611	2616	rBB	286	196	0.02%	0.003%
68	9.796	2624	2630	2632	rBV	221	257	0.03%	0.004%
69	9.896	2658	2661	2663	rBV	188	148	0.02%	0.002%
70	9.922	2667	2669	2673	rVB2	359	267	0.03%	0.004%
71	10.031	2696	2703	2706	rBV	261	368	0.04%	0.005%
72	10.095	2720	2723	2725	rBV2	251	214	0.03%	0.003%
73	10.121	2729	2731	2735	rBV	301	188	0.02%	0.003%
74	10.179	2746	2749	2751	rBV2	235	163	0.02%	0.002%
75	10.218	2758	2761	2764	rBV	256	249	0.03%	0.004%
76	10.266	2773	2776	2779	rBV	214	202	0.02%	0.003%

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

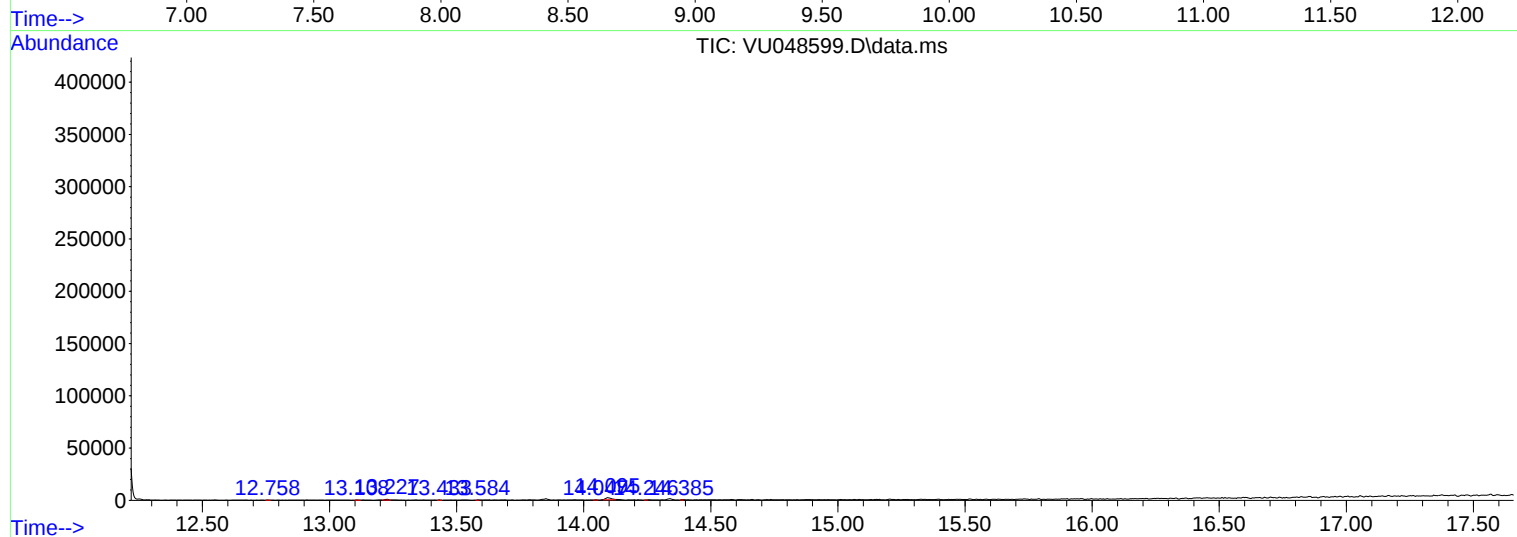
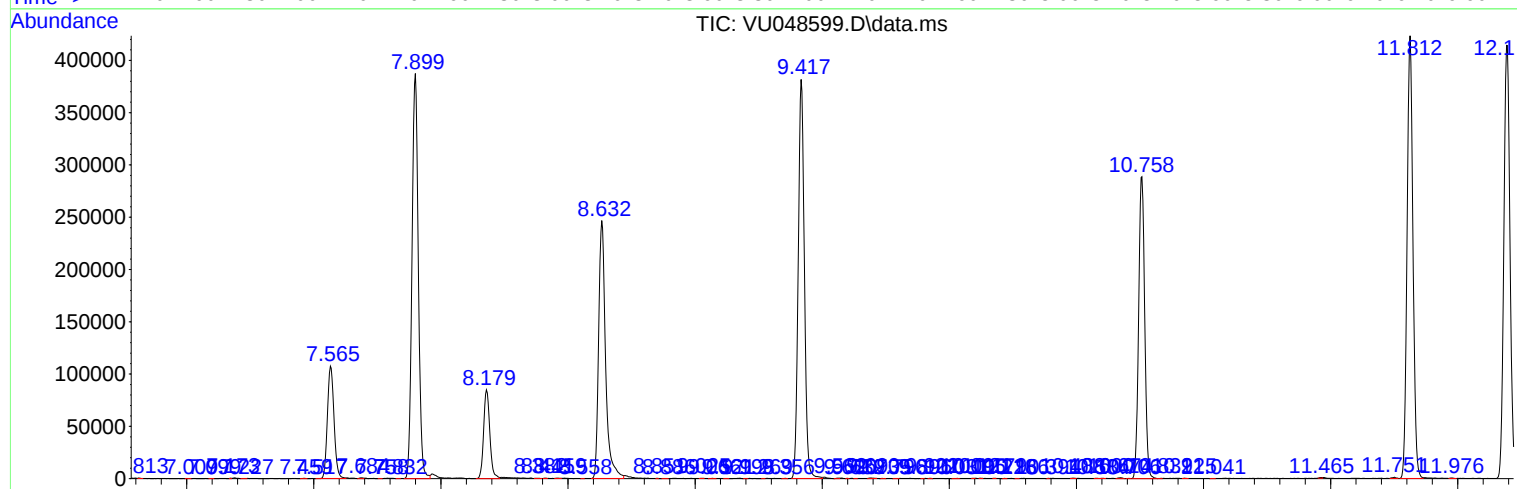
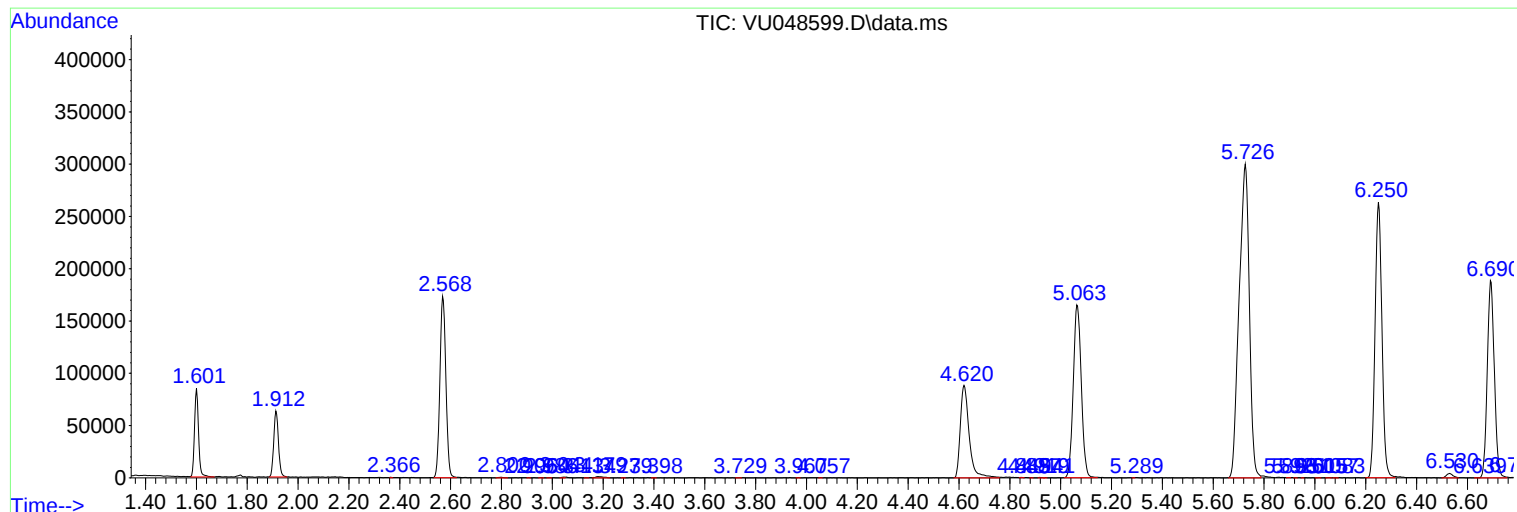
77	10.391	2812	2815	2816	rBV	315	191	0.02%	0.003%
78	10.488	2841	2845	2849	rBV	350	366	0.04%	0.005%
79	10.584	2870	2875	2877	rBV2	199	184	0.02%	0.003%
80	10.600	2877	2880	2885	rVV2	191	173	0.02%	0.003%
81	10.674	2897	2903	2908	rVB3	867	1036	0.12%	0.015%
82	10.706	2909	2913	2916	rBV	304	248	0.03%	0.004%
83	10.758	2917	2929	2948	rVB	288694	473201	56.52%	7.061%
84	10.832	2948	2952	2954	rBV	327	224	0.03%	0.003%
85	10.925	2978	2981	2986	rVB2	326	236	0.03%	0.004%
86	11.041	3012	3017	3019	rBV	211	258	0.03%	0.004%
87	11.465	3144	3149	3150	rBV	718	619	0.07%	0.009%
88	11.751	3232	3238	3243	rVB3	1108	1119	0.13%	0.017%
89	11.812	3244	3257	3273	rBV	423319	671810	80.24%	10.024%
90	11.976	3304	3308	3314	rVB2	578	552	0.07%	0.008%
91	12.192	3363	3375	3391	rBV	414099	689730	82.38%	10.291%
92	12.758	3548	3551	3554	rBV	283	159	0.02%	0.002%
93	13.108	3657	3660	3664	rVV2	215	162	0.02%	0.002%
94	13.227	3691	3697	3701	rBV3	705	754	0.09%	0.011%
95	13.433	3758	3761	3764	rVB2	361	217	0.03%	0.003%
96	13.584	3805	3808	3809	rBV	361	189	0.02%	0.003%
97	14.047	3949	3952	3955	rBV	357	216	0.03%	0.003%
98	14.095	3961	3967	3976	rBV2	1876	2941	0.35%	0.044%
99	14.246	4011	4014	4015	rBV	285	188	0.02%	0.003%
100	14.385	4055	4057	4059	rBV	462	287	0.03%	0.004%

Sum of corrected areas: 6702028

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

No Library Search Compounds Detected

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