

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041123\
 Data File : VU053649.D
 Acq On : 11 Apr 2023 20:44
 Operator : JC/MD
 Sample : 02252-09 200X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COME5

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053649.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	73	80	90	rBV	87294	98603	13.01%	1.612%
2	1.909	169	177	196	rVB	76031	109518	14.46%	1.791%
3	2.565	370	381	395	rVB	140798	227255	30.00%	3.716%
4	3.044	521	530	541	rVB4	1722	3374	0.45%	0.055%
5	3.372	628	632	639	rVB2	227	248	0.03%	0.004%
6	3.465	660	661	662	rBV2	155	53	0.01%	0.001%
7	3.668	716	724	727	rBV	368	430	0.06%	0.007%
8	3.713	735	738	742	rVB2	233	153	0.02%	0.003%
9	3.829	772	774	778	rBV	235	153	0.02%	0.003%
10	3.980	818	821	827	rBV	233	201	0.03%	0.003%
11	4.018	831	833	836	rVB	155	54	0.01%	0.001%
12	4.105	856	860	867	rVB2	342	442	0.06%	0.007%
13	4.144	867	872	876	rBV2	279	342	0.05%	0.006%
14	4.558	999	1001	1004	rBV	245	162	0.02%	0.003%
15	4.613	1007	1018	1041	rBV	65434	158112	20.87%	2.585%
16	5.057	1140	1156	1174	rBV	139215	301707	39.82%	4.933%
17	5.456	1277	1280	1283	rBV	244	205	0.03%	0.003%
18	5.719	1341	1362	1403	rBV2	266001	757627	100.00%	12.388%
19	5.938	1427	1430	1433	rBV	361	174	0.02%	0.003%
20	5.976	1439	1442	1444	rVB	219	95	0.01%	0.002%
21	6.009	1450	1452	1457	rBV2	219	155	0.02%	0.003%
22	6.047	1460	1464	1468	rBV2	296	246	0.03%	0.004%
23	6.243	1511	1525	1549	rBV	265402	505886	66.77%	8.271%
24	6.456	1586	1591	1594	rBV2	280	306	0.04%	0.005%
25	6.526	1605	1613	1623	rVB5	2821	5212	0.69%	0.085%
26	6.587	1629	1632	1634	rBV	194	137	0.02%	0.002%
27	6.684	1647	1662	1682	rBV	171499	332986	43.95%	5.444%
28	6.851	1712	1714	1716	rBV	144	52	0.01%	0.001%
29	6.890	1723	1726	1729	rBV	269	155	0.02%	0.003%
30	6.931	1736	1739	1744	rBV	182	180	0.02%	0.003%
31	6.954	1744	1746	1751	rBV	190	152	0.02%	0.002%
32	7.012	1760	1764	1768	rBV	162	135	0.02%	0.002%
33	7.037	1768	1772	1777	rVV2	273	250	0.03%	0.004%
34	7.121	1795	1798	1799	rBV	190	130	0.02%	0.002%
35	7.182	1811	1817	1820	rBV3	978	1075	0.14%	0.018%
36	7.230	1828	1832	1834	rBV	329	256	0.03%	0.004%

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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\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.308	1852	1856	1861	rBV2	187	218	0.03%	0.004%
38	7.333	1861	1864	1867	rBV	203	175	0.02%	0.003%
39	7.382	1876	1879	1882	rVB2	226	156	0.02%	0.003%
40	7.439	1895	1897	1902	rVB	242	156	0.02%	0.003%
41	7.513	1918	1920	1922	rBV	189	91	0.01%	0.001%
42	7.562	1923	1935	1955	rVV	93780	162771	21.48%	2.661%
43	7.687	1969	1974	1979	rBV3	905	1091	0.14%	0.018%
44	7.738	1988	1990	1993	rBB	178	49	0.01%	0.001%
45	7.893	2025	2038	2060	rBV	339231	589187	77.77%	9.634%
46	8.099	2100	2102	2104	rVB	345	128	0.02%	0.002%
47	8.176	2114	2126	2144	rBV2	64702	108713	14.35%	1.778%
48	8.288	2157	2161	2163	rBV3	311	279	0.04%	0.005%
49	8.330	2171	2174	2176	rVB	304	146	0.02%	0.002%
50	8.401	2193	2196	2198	rBV	196	123	0.02%	0.002%
51	8.558	2238	2245	2248	rBV	310	429	0.06%	0.007%
52	8.626	2256	2266	2301	rVB	199791	359300	47.42%	5.875%
53	8.864	2338	2340	2344	rVB2	275	163	0.02%	0.003%
54	8.925	2356	2359	2362	rBV	285	234	0.03%	0.004%
55	8.973	2371	2374	2382	rVB2	178	205	0.03%	0.003%
56	9.005	2382	2384	2387	rBV	259	164	0.02%	0.003%
57	9.182	2437	2439	2442	rBV	198	152	0.02%	0.002%
58	9.282	2468	2470	2474	rVB	301	160	0.02%	0.003%
59	9.356	2488	2493	2496	rBV2	255	254	0.03%	0.004%
60	9.414	2498	2511	2543	rVV	365913	675671	89.18%	11.048%
61	9.761	2617	2619	2620	rBV	173	56	0.01%	0.001%
62	9.893	2657	2660	2665	rBV	165	116	0.02%	0.002%
63	10.018	2696	2699	2701	rBV	254	156	0.02%	0.003%
64	10.471	2835	2840	2841	rBV	249	203	0.03%	0.003%
65	10.751	2914	2927	2943	rBV	264466	422595	55.78%	6.910%
66	11.079	3024	3029	3030	rBV	366	316	0.04%	0.005%
67	11.163	3053	3055	3056	rBV	170	57	0.01%	0.001%
68	11.317	3102	3103	3104	rBV	186	49	0.01%	0.001%
69	11.343	3108	3111	3120	rVB2	328	360	0.05%	0.006%
70	11.523	3165	3167	3169	rBV2	193	105	0.01%	0.002%
71	11.671	3209	3213	3214	rBV	437	271	0.04%	0.004%
72	11.809	3244	3256	3278	rBV	394253	670790	88.54%	10.968%
73	12.188	3361	3374	3396	rBV	362218	610017	80.52%	9.974%
74	12.372	3429	3431	3432	rBV	249	123	0.02%	0.002%
75	13.410	3750	3754	3757	rBV2	315	236	0.03%	0.004%
76	13.793	3871	3873	3874	rBV	394	186	0.02%	0.003%

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C0ME5

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\SFAMULM033123WMA.M
Title : VOC Analysis

77	13.847	3883	3890	3897	rBV5	2262	3539	0.47%	0.058%
78	13.999	3934	3937	3939	rBV	307	253	0.03%	0.004%
79	14.420	4065	4068	4071	rBV3	426	355	0.05%	0.006%

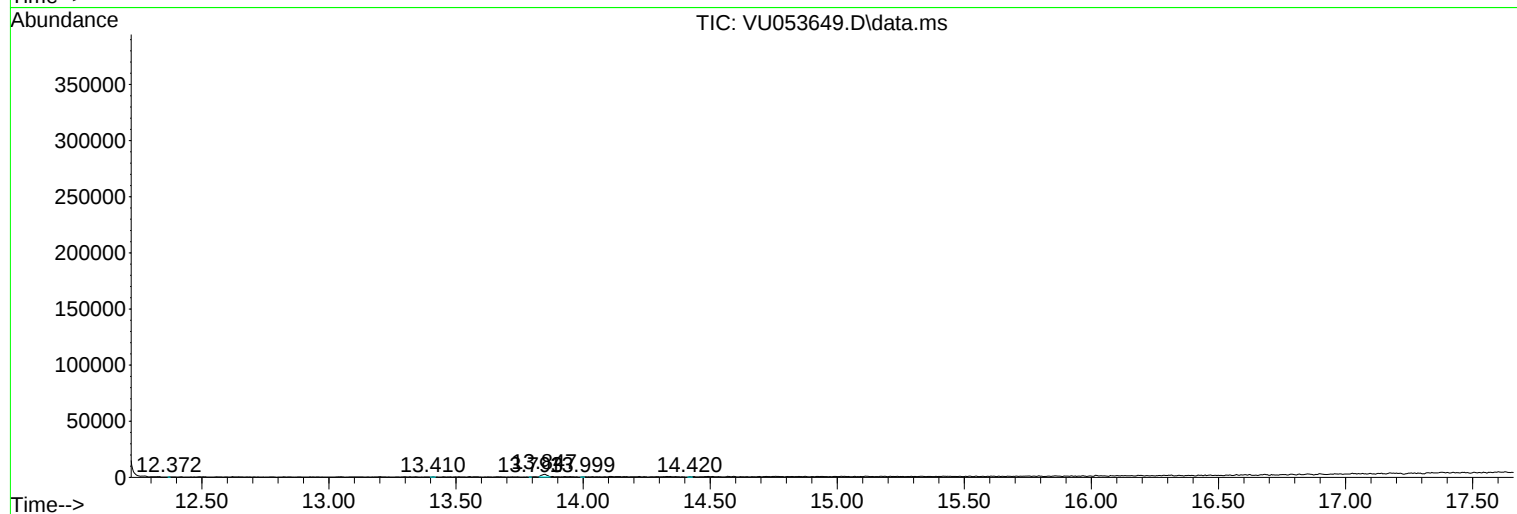
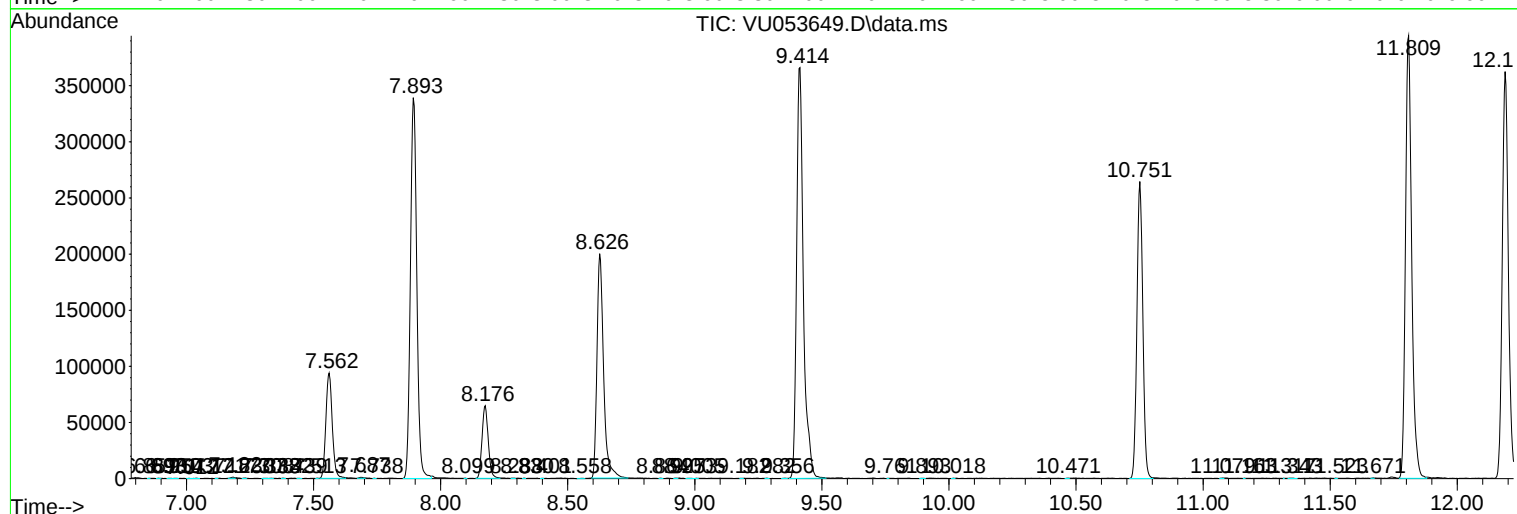
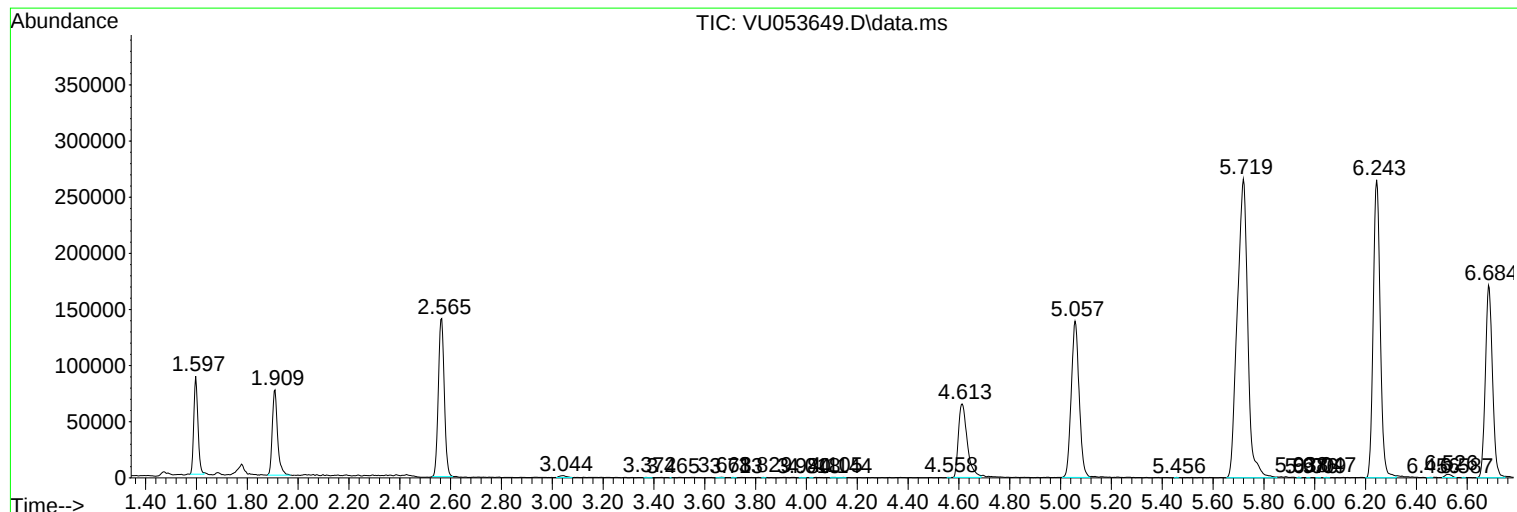
Sum of corrected areas: 6116019

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



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MSVOA_U
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C0ME5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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\SFAMULM033123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc