

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100322\  
 Data File : VU051097.D  
 Acq On : 03 Oct 2022 20:58  
 Operator : JC/MD  
 Sample : N4880-13  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGS2

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092922WMA.M  
 Title : VOC Analysis

Signal : TIC: VU051097.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	96	rBV	204676	256373	16.23%	2.248%
2	1.903	167	175	199	rVB	173633	237746	15.05%	2.084%
3	2.565	368	381	395	rBV	302108	493037	31.22%	4.323%
4	2.668	411	413	416	rVB	768	378	0.02%	0.003%
5	2.736	432	434	438	rBV	606	470	0.03%	0.004%
6	2.771	438	445	449	rBV6	1279	1670	0.11%	0.015%
7	2.851	467	470	471	rBV2	563	361	0.02%	0.003%
8	3.022	520	523	525	rBV2	590	349	0.02%	0.003%
9	3.048	525	531	534	rBV5	1226	1332	0.08%	0.012%
10	3.089	539	544	546	rBV	419	417	0.03%	0.004%
11	3.128	552	556	560	rBV3	512	353	0.02%	0.003%
12	3.179	560	572	574	rBV6	3434	5554	0.35%	0.049%
13	3.411	639	644	648	rBV	589	460	0.03%	0.004%
14	3.495	666	670	677	rVB3	643	763	0.05%	0.007%
15	3.662	718	722	725	rBV3	455	363	0.02%	0.003%
16	3.777	751	758	762	rBV3	303	386	0.02%	0.003%
17	3.832	770	775	778	rBB3	481	384	0.02%	0.003%
18	3.964	809	816	822	rVB	583	876	0.06%	0.008%
19	4.089	850	855	858	rBV2	400	460	0.03%	0.004%
20	4.183	881	884	887	rBV3	449	347	0.02%	0.003%
21	4.257	904	907	913	rVB2	490	388	0.02%	0.003%
22	4.372	938	943	947	rBV3	399	464	0.03%	0.004%
23	4.466	969	972	976	rBV2	419	358	0.02%	0.003%
24	4.617	1007	1019	1050	rBV	146591	376472	23.84%	3.301%
25	5.060	1139	1157	1183	rBV	293375	646969	40.97%	5.672%
26	5.189	1194	1197	1201	rVB5	525	347	0.02%	0.003%
27	5.282	1224	1226	1229	rBV2	853	450	0.03%	0.004%
28	5.626	1327	1333	1337	rBV3	550	483	0.03%	0.004%
29	5.723	1341	1363	1386	rBV2	577743	1579201	100.00%	13.845%
30	6.041	1459	1462	1466	rBV3	583	388	0.02%	0.003%
31	6.105	1479	1482	1487	rBV3	583	539	0.03%	0.005%
32	6.186	1501	1507	1511	rVB2	249	343	0.02%	0.003%
33	6.247	1511	1526	1550	rBV	440019	829657	52.54%	7.274%
34	6.527	1604	1613	1624	rBV6	9401	18842	1.19%	0.165%
35	6.629	1641	1645	1647	rBV3	513	362	0.02%	0.003%
36	6.687	1648	1663	1690	rVV	380338	744160	47.12%	6.524%

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100322\  
 Data File : VU051097.D  
 Acq On : 03 Oct 2022 20:58  
 Operator : JC/MD  
 Sample : N4880-13  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGS2

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092922WMA.M  
 Title : VOC Analysis

37	6.909	1728	1732	1736	rVB4	830	784	0.05%	0.007%
38	7.025	1762	1768	1771	rBV2	555	492	0.03%	0.004%
39	7.163	1807	1811	1812	rBV	618	421	0.03%	0.004%
40	7.234	1829	1833	1838	rBV2	348	413	0.03%	0.004%
41	7.285	1845	1849	1854	rBV2	407	395	0.03%	0.003%
42	7.321	1855	1860	1865	rVB2	350	376	0.02%	0.003%
43	7.382	1871	1879	1881	rBV2	300	349	0.02%	0.003%
44	7.565	1923	1936	1954	rBV	177153	315043	19.95%	2.762%
45	7.694	1973	1976	1978	rBV3	657	500	0.03%	0.004%
46	7.729	1984	1987	1994	rVB2	653	652	0.04%	0.006%
47	7.764	1994	1998	2003	rBV3	465	451	0.03%	0.004%
48	7.803	2004	2010	2013	rVV3	384	338	0.02%	0.003%
49	7.896	2025	2039	2060	rBV	639306	1098662	69.57%	9.632%
50	8.118	2105	2108	2112	rBV2	558	480	0.03%	0.004%
51	8.176	2115	2126	2143	rVV	125194	212527	13.46%	1.863%
52	8.462	2211	2215	2216	rBV3	588	354	0.02%	0.003%
53	8.472	2216	2218	2222	rVB4	446	340	0.02%	0.003%
54	8.552	2231	2243	2256	rBV2	71553	120398	7.62%	1.056%
55	8.633	2256	2268	2302	rBV3	363237	819304	51.88%	7.183%
56	8.880	2342	2345	2349	rVB3	652	441	0.03%	0.004%
57	8.986	2373	2378	2384	rBV2	521	622	0.04%	0.005%
58	9.041	2390	2395	2400	rBV3	566	764	0.05%	0.007%
59	9.102	2409	2414	2422	rVB2	441	575	0.04%	0.005%
60	9.163	2431	2433	2440	rBV3	313	347	0.02%	0.003%
61	9.414	2498	2511	2530	rBV	640231	1058805	67.05%	9.283%
62	9.694	2593	2598	2603	rBV3	705	669	0.04%	0.006%
63	9.774	2620	2623	2628	rVV2	454	374	0.02%	0.003%
64	9.967	2680	2683	2686	rBV	375	337	0.02%	0.003%
65	10.028	2699	2702	2707	rBV2	377	382	0.02%	0.003%
66	10.436	2824	2829	2833	rBV3	474	484	0.03%	0.004%
67	10.536	2856	2860	2862	rBV	532	336	0.02%	0.003%
68	10.755	2914	2928	2950	rBV	543789	873577	55.32%	7.659%
69	10.883	2965	2968	2971	rBV2	613	500	0.03%	0.004%
70	11.105	3035	3037	3048	rVB4	918	1114	0.07%	0.010%
71	11.356	3112	3115	3120	rVB2	553	442	0.03%	0.004%
72	11.382	3120	3123	3127	rBV	534	520	0.03%	0.005%
73	11.523	3164	3167	3174	rVB3	463	488	0.03%	0.004%
74	11.687	3214	3218	3223	rBV4	1180	1258	0.08%	0.011%
75	11.742	3227	3235	3237	rBV2	564	539	0.03%	0.005%
76	11.809	3243	3256	3281	rBV	476121	759972	48.12%	6.663%

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100322\  
 Data File : VU051097.D  
 Acq On : 03 Oct 2022 20:58  
 Operator : JC/MD  
 Sample : N4880-13  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGS2

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092922WMA.M  
 Title : VOC Analysis

77	12.002	3312	3316	3323	rBV4	528	537	0.03%	0.005%
78	12.067	3330	3336	3350	rVB6	4486	8815	0.56%	0.077%
79	12.121	3350	3353	3359	rVB3	895	944	0.06%	0.008%
80	12.192	3359	3375	3406	rBV	544900	906367	57.39%	7.946%
81	12.343	3420	3422	3428	rVB4	884	673	0.04%	0.006%
82	12.378	3430	3433	3435	rBV	562	332	0.02%	0.003%
83	12.719	3536	3539	3543	rBV3	684	570	0.04%	0.005%
84	12.800	3561	3564	3567	rBV3	585	446	0.03%	0.004%
85	12.893	3590	3593	3600	rVB6	1876	2005	0.13%	0.018%
86	13.169	3675	3679	3680	rBV2	582	453	0.03%	0.004%
87	13.195	3685	3687	3690	rVB3	617	371	0.02%	0.003%
88	13.214	3690	3693	3695	rBV2	551	369	0.02%	0.003%
89	13.353	3732	3736	3738	rBV2	699	485	0.03%	0.004%
90	13.407	3750	3753	3757	rVB	629	436	0.03%	0.004%
91	13.439	3757	3763	3767	rBV2	500	608	0.04%	0.005%
92	13.491	3775	3779	3786	rVB2	643	563	0.04%	0.005%
93	13.526	3786	3790	3792	rBV2	793	600	0.04%	0.005%
94	13.684	3835	3839	3842	rBV3	624	640	0.04%	0.006%
95	14.208	3999	4002	4005	rVB2	618	338	0.02%	0.003%
96	14.320	4034	4037	4046	rVB4	910	1289	0.08%	0.011%
97	14.369	4047	4052	4057	rBV4	909	1058	0.07%	0.009%
98	14.394	4057	4060	4065	rVV2	527	417	0.03%	0.004%
99	14.420	4066	4068	4073	rVB2	761	582	0.04%	0.005%
100	15.545	4415	4418	4422	rVB2	1281	960	0.06%	0.008%

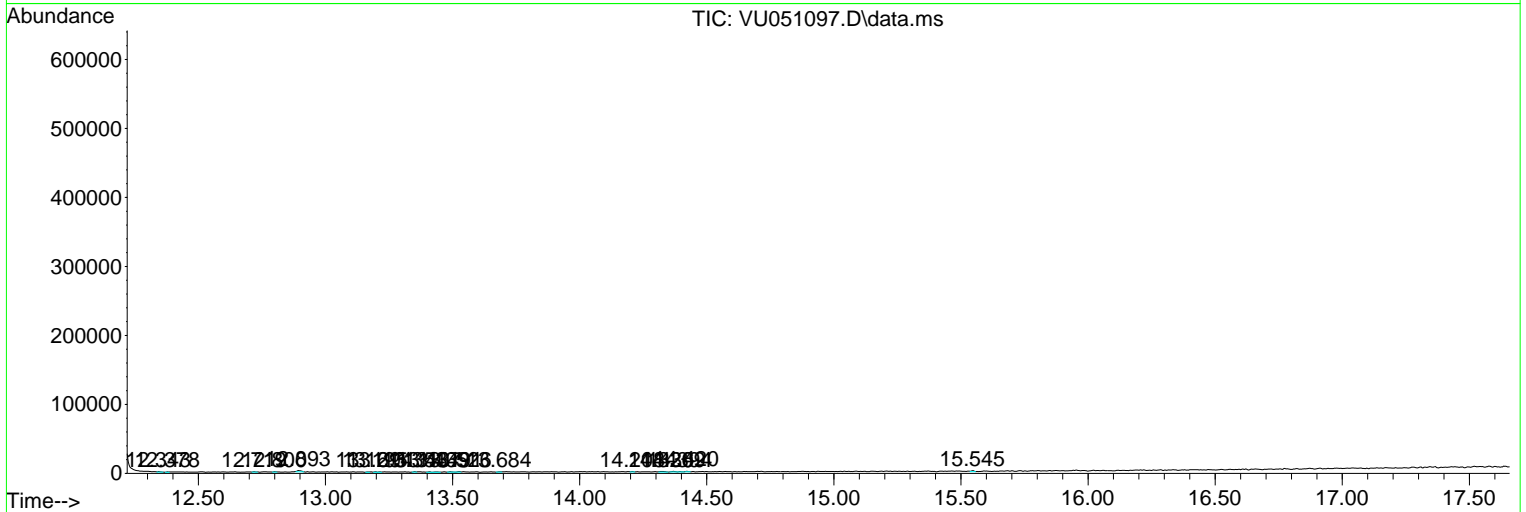
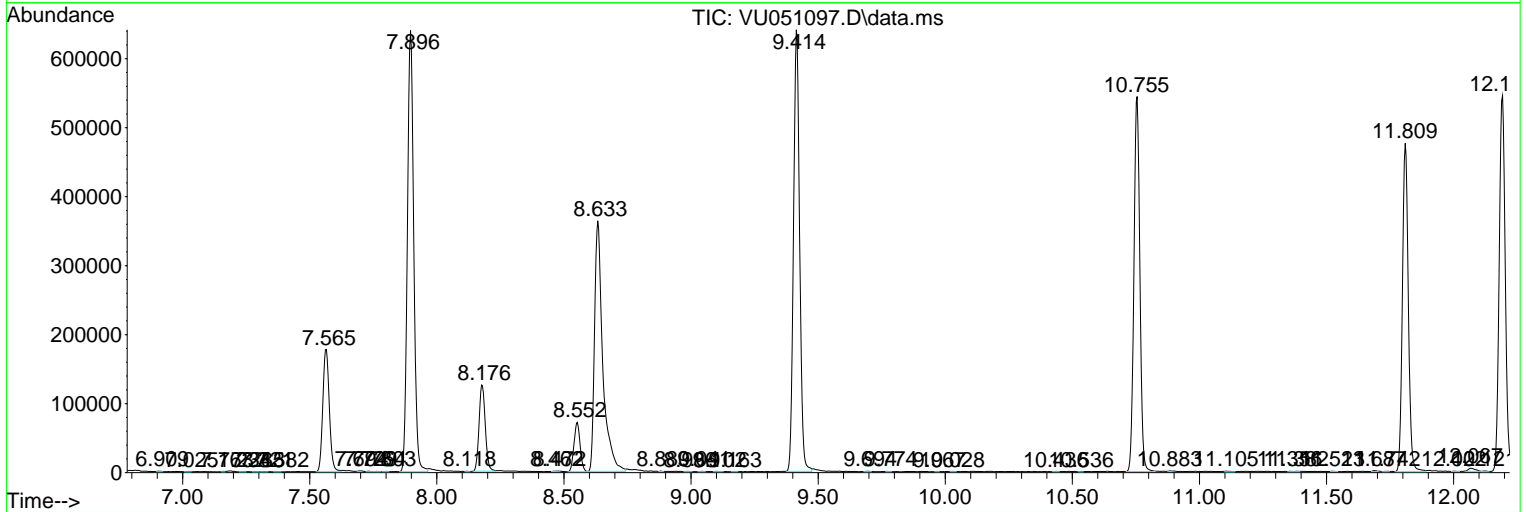
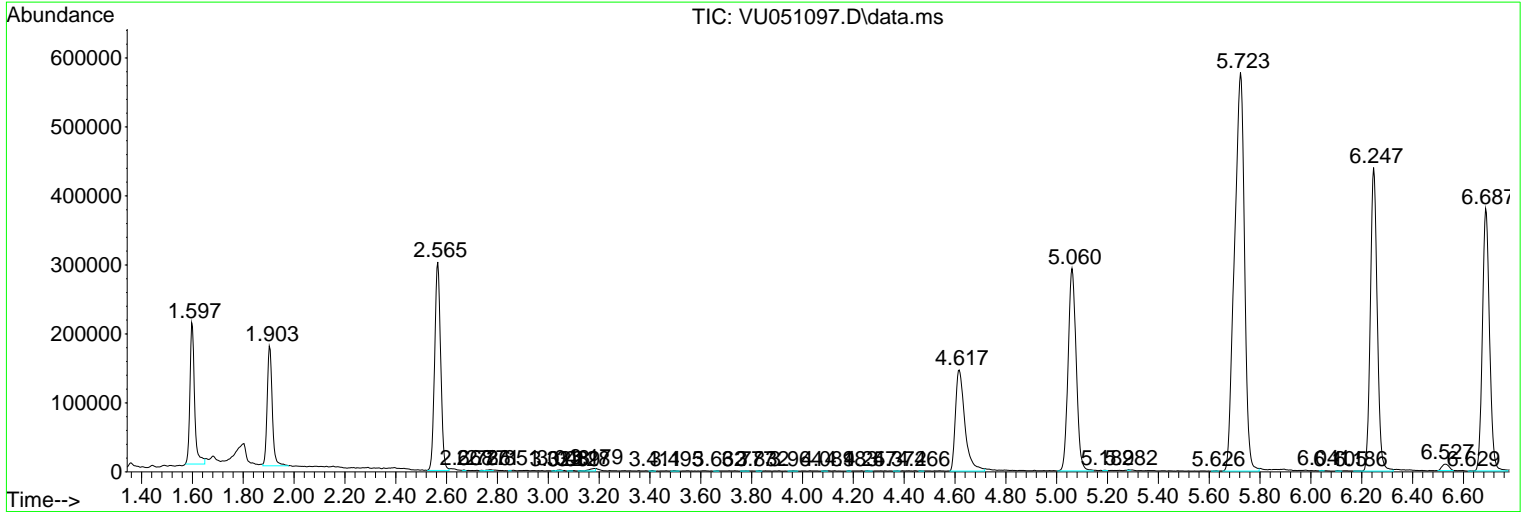
Sum of corrected areas: 11406185

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100322\  
 Data File : VU051097.D  
 Acq On : 03 Oct 2022 20:58  
 Operator : JC/MD  
 Sample : N4880-13  
 Misc : 5.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BGS2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092922WMA.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\VU100322\  
Data File : VU051097.D  
Acq On : 03 Oct 2022 20:58  
Operator : JC/MD  
Sample : N4880-13  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BGSG2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092922WMA.M  
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

\*\*\*\*\*

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU100322\  
Data File : VU051097.D  
Acq On : 03 Oct 2022 20:58  
Operator : JC/MD  
Sample : N4880-13  
Misc : 5.0mL/MSVOA\_U/WATER  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
MSVOA\_U  
ClientSampleId :  
BGS2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMULM092922WMA.M  
Quant Title : VOC Analysis

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

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

---