

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092722\
 Data File : VU050952.D
 Acq On : 27 Sep 2022 12:38
 Operator : JC/MD
 Sample : VU0927MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK189

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\SFAMULM092022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050952.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	100	rVB	182362	215560	12.68%	1.667%
2	1.912	169	178	191	rBV	167924	218527	12.86%	1.690%
3	2.568	369	382	397	rBV	310019	508001	29.89%	3.929%
4	2.684	415	418	421	rVB	671	426	0.03%	0.003%
5	2.790	444	451	453	rBV4	928	1159	0.07%	0.009%
6	2.941	492	498	501	rBV3	573	656	0.04%	0.005%
7	2.996	512	515	519	rBV2	304	256	0.02%	0.002%
8	3.047	519	531	545	rVV3	14605	27679	1.63%	0.214%
9	3.182	560	573	589	rVB	15232	34454	2.03%	0.266%
10	3.330	612	619	623	rBV2	321	288	0.02%	0.002%
11	3.356	624	627	629	rBV2	365	261	0.02%	0.002%
12	3.388	635	637	642	rVB	387	246	0.01%	0.002%
13	3.481	663	666	674	rBV	427	496	0.03%	0.004%
14	3.575	691	695	697	rVB2	371	224	0.01%	0.002%
15	3.996	823	826	832	rVB2	288	275	0.02%	0.002%
16	4.240	894	902	907	rVB2	504	700	0.04%	0.005%
17	4.288	909	917	922	rBV2	243	373	0.02%	0.003%
18	4.321	922	927	931	rBV2	205	219	0.01%	0.002%
19	4.456	965	969	974	rBV	331	321	0.02%	0.002%
20	4.616	1005	1019	1049	rBV	222332	548902	32.29%	4.245%
21	4.973	1127	1130	1133	rBV2	411	261	0.02%	0.002%
22	5.063	1140	1158	1184	rBV	319762	699355	41.15%	5.409%
23	5.285	1221	1227	1228	rBV2	800	757	0.04%	0.006%
24	5.337	1240	1243	1246	rBV2	412	270	0.02%	0.002%
25	5.382	1250	1257	1263	rVV5	826	994	0.06%	0.008%
26	5.443	1270	1276	1279	rVB2	282	256	0.02%	0.002%
27	5.726	1341	1364	1384	rBV2	622216	1699703	100.00%	13.145%
28	5.931	1426	1428	1433	rBV2	432	431	0.03%	0.003%
29	6.028	1455	1458	1459	rBV	697	348	0.02%	0.003%
30	6.118	1481	1486	1490	rBV3	626	568	0.03%	0.004%
31	6.250	1510	1527	1552	rBV	443537	853752	50.23%	6.603%
32	6.365	1561	1563	1567	rVB4	1081	835	0.05%	0.006%
33	6.414	1575	1578	1583	rVB4	515	504	0.03%	0.004%
34	6.484	1594	1600	1602	rBV2	422	485	0.03%	0.004%
35	6.529	1603	1614	1631	rVB4	16739	32689	1.92%	0.253%
36	6.623	1641	1643	1646	rVB	428	259	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092722\
 Data File : VU050952.D
 Acq On : 27 Sep 2022 12:38
 Operator : JC/MD
 Sample : VU0927MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK189

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\SFAMULM092022WMA.M
 Title : VOC Analysis

37	6.690	1649	1664	1688	rBV	418334	812315	47.79%	6.282%
38	6.806	1693	1700	1712	rVV8	2146	4867	0.29%	0.038%
39	6.867	1716	1719	1725	rVB5	755	721	0.04%	0.006%
40	7.092	1785	1789	1792	rVV	328	237	0.01%	0.002%
41	7.134	1799	1802	1806	rVB	349	234	0.01%	0.002%
42	7.192	1811	1820	1828	rVV5	2039	3647	0.21%	0.028%
43	7.253	1837	1839	1845	rVB2	327	260	0.02%	0.002%
44	7.298	1845	1853	1857	rBV2	555	773	0.05%	0.006%
45	7.430	1889	1894	1897	rBV2	205	220	0.01%	0.002%
46	7.510	1911	1919	1922	rBV2	318	329	0.02%	0.003%
47	7.565	1923	1936	1959	rBV	207321	364399	21.44%	2.818%
48	7.690	1971	1975	1980	rVV4	1319	1187	0.07%	0.009%
49	7.761	1993	1997	1999	rBV3	258	219	0.01%	0.002%
50	7.790	2002	2006	2008	rBV4	889	792	0.05%	0.006%
51	7.899	2025	2040	2056	rBV	715244	1236880	72.77%	9.566%
52	8.057	2087	2089	2093	rVB	467	306	0.02%	0.002%
53	8.131	2108	2112	2115	rBV3	888	689	0.04%	0.005%
54	8.179	2115	2127	2144	rBV	154717	256212	15.07%	1.982%
55	8.552	2239	2243	2247	rBV3	771	665	0.04%	0.005%
56	8.632	2255	2268	2303	rBV3	528578	1104819	65.00%	8.545%
57	8.880	2343	2345	2350	rVB4	628	396	0.02%	0.003%
58	8.912	2353	2355	2358	rVV2	617	324	0.02%	0.003%
59	8.931	2359	2361	2365	rVB2	600	295	0.02%	0.002%
60	8.989	2376	2379	2382	rVB2	634	393	0.02%	0.003%
61	9.018	2385	2388	2391	rVB2	486	223	0.01%	0.002%
62	9.079	2405	2407	2411	rVV2	385	232	0.01%	0.002%
63	9.417	2499	2512	2550	rVV	678335	1118506	65.81%	8.650%
64	9.565	2550	2558	2563	rVV5	1012	1548	0.09%	0.012%
65	9.648	2579	2584	2589	rVB2	595	654	0.04%	0.005%
66	9.693	2593	2598	2607	rBV4	1528	2118	0.12%	0.016%
67	9.780	2619	2625	2627	rBV	367	346	0.02%	0.003%
68	9.922	2666	2669	2672	rVB	495	279	0.02%	0.002%
69	10.098	2719	2724	2726	rBV2	676	494	0.03%	0.004%
70	10.150	2737	2740	2746	rVB3	449	378	0.02%	0.003%
71	10.182	2746	2750	2754	rBV2	295	307	0.02%	0.002%
72	10.433	2825	2828	2830	rBV	406	281	0.02%	0.002%
73	10.488	2840	2845	2854	rVV3	750	845	0.05%	0.007%
74	10.642	2887	2893	2898	rVV3	1354	2036	0.12%	0.016%
75	10.668	2898	2901	2908	rVB5	1957	2218	0.13%	0.017%
76	10.754	2915	2928	2945	rBV	635237	1017673	59.87%	7.871%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092722\
 Data File : VU050952.D
 Acq On : 27 Sep 2022 12:38
 Operator : JC/MD
 Sample : VU0927MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK189

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\SFAMULM092022WMA.M
 Title : VOC Analysis

77	11.089	3024	3032	3037	rBV3	908	1230	0.07%	0.010%
78	11.143	3046	3049	3050	rBV	444	284	0.02%	0.002%
79	11.362	3114	3117	3121	rBV2	306	249	0.01%	0.002%
80	11.407	3126	3131	3134	rBV3	437	421	0.02%	0.003%
81	11.465	3140	3149	3158	rBV8	1532	3013	0.18%	0.023%
82	11.690	3216	3219	3220	rBV	405	219	0.01%	0.002%
83	11.741	3231	3235	3244	rBV4	1905	2622	0.15%	0.020%
84	11.812	3244	3257	3287	rBV	594868	941393	55.39%	7.281%
85	11.970	3302	3306	3307	rBV3	948	704	0.04%	0.005%
86	11.995	3312	3314	3317	rVB3	408	234	0.01%	0.002%
87	12.192	3358	3375	3398	rBV	714013	1169693	68.82%	9.046%
88	12.352	3422	3425	3429	rBV3	460	428	0.03%	0.003%
89	12.436	3448	3451	3452	rBV2	438	239	0.01%	0.002%
90	12.587	3496	3498	3501	rVB2	462	222	0.01%	0.002%
91	13.002	3622	3627	3629	rBV	620	659	0.04%	0.005%
92	13.221	3692	3695	3708	rVB5	2005	3343	0.20%	0.026%
93	13.272	3708	3711	3713	rBV2	530	348	0.02%	0.003%
94	13.343	3727	3733	3734	rBV2	621	587	0.03%	0.005%
95	13.388	3745	3747	3749	rBV	540	352	0.02%	0.003%
96	13.844	3883	3889	3897	rVB7	2530	3952	0.23%	0.031%
97	14.092	3958	3966	3976	rBV2	3357	5531	0.33%	0.043%
98	14.336	4035	4042	4049	rBV5	2632	3861	0.23%	0.030%
99	15.069	4268	4270	4272	rBV2	481	261	0.02%	0.002%
100	15.735	4475	4477	4478	rBV2	943	453	0.03%	0.004%

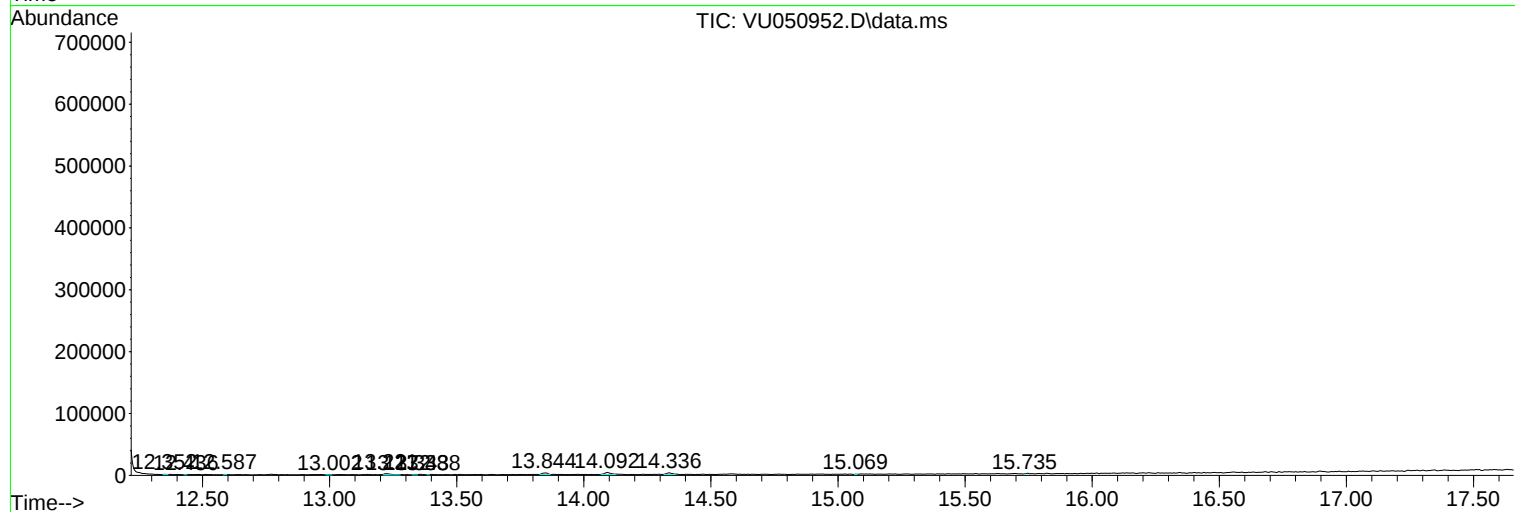
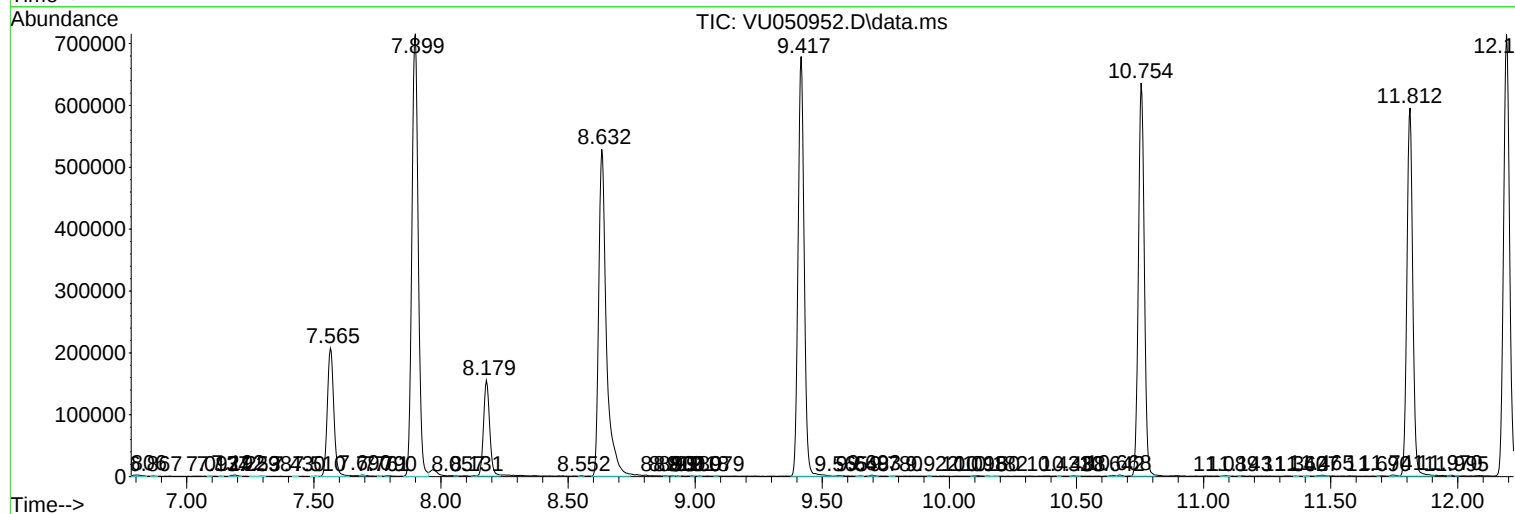
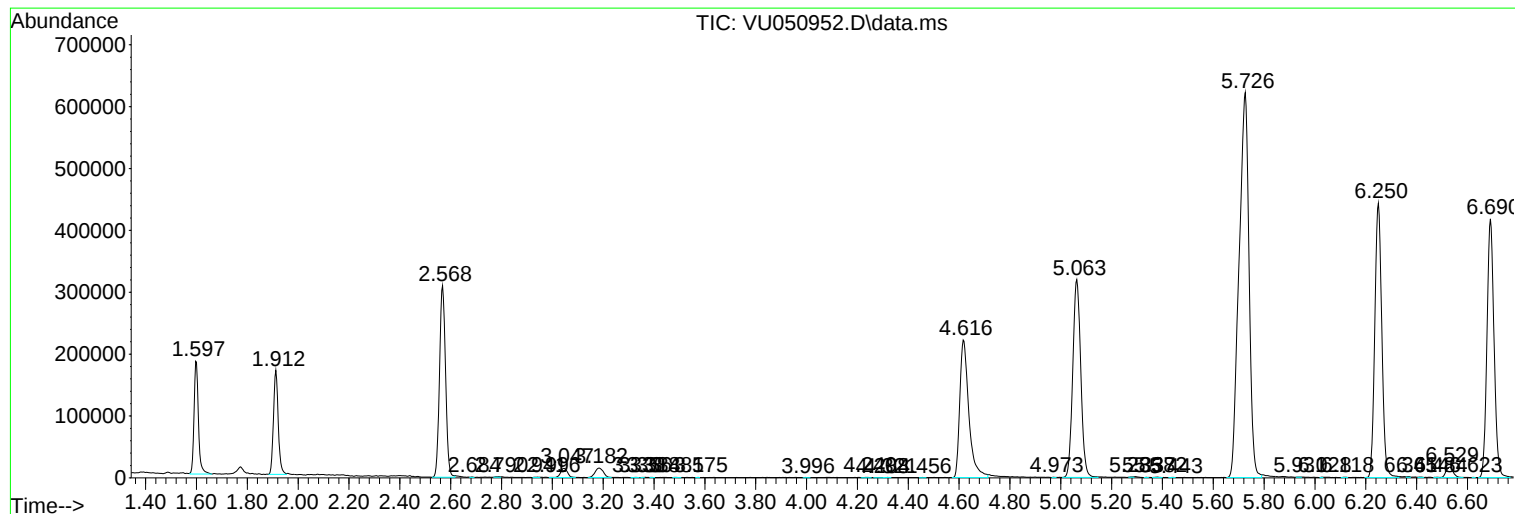
Sum of corrected areas: 12930105

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092722\
Data File : VU050952.D
Acq On : 27 Sep 2022 12:38
Operator : JC/MD
Sample : VU0927MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK189

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092722\
Data File : VU050952.D
Acq On : 27 Sep 2022 12:38
Operator : JC/MD
Sample : VU0927MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK189

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092722\
Data File : VU050952.D
Acq On : 27 Sep 2022 12:38
Operator : JC/MD
Sample : VU0927MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK189

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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