

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059380.D
 Acq On : 20 Jun 2024 15:10
 Operator : MD/SY
 Sample : P2960-14
 Misc : 5.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB51

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\SFAMULM052924WMA.M

Title : VOC Analysis

Signal : TIC: VU059380.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.592	87	94	116	rVB	35095	58516	7.94%	1.086%
2	1.821	135	165	167	rBV5	43191	154579	20.97%	2.870%
3	2.535	376	387	409	rVB	91319	149283	20.25%	2.771%
4	2.634	415	418	425	rVB5	638	596	0.08%	0.011%
5	2.911	502	504	508	rVB2	366	282	0.04%	0.005%
6	3.023	530	539	558	rVB4	3551	8456	1.15%	0.157%
7	3.097	558	562	566	rBV2	288	269	0.04%	0.005%
8	3.178	577	587	597	rVV3	747	1561	0.21%	0.029%
9	3.377	642	649	650	rBV	342	290	0.04%	0.005%
10	3.834	788	791	797	rVB	294	330	0.04%	0.006%
11	4.049	854	858	862	rBV2	354	356	0.05%	0.007%
12	4.506	995	1000	1003	rBV2	298	313	0.04%	0.006%
13	4.624	1026	1037	1081	rBV2	45335	141516	19.20%	2.627%
14	4.927	1127	1131	1139	rVB2	395	559	0.08%	0.010%
15	4.962	1139	1142	1145	rBV2	319	268	0.04%	0.005%
16	5.052	1152	1170	1191	rBV	92093	208882	28.34%	3.878%
17	5.441	1288	1291	1296	rVB2	227	244	0.03%	0.005%
18	5.711	1356	1375	1397	rBV2	195763	517262	70.17%	9.602%
19	5.972	1451	1456	1459	rBV3	841	854	0.12%	0.016%
20	6.100	1490	1496	1500	rBV2	408	475	0.06%	0.009%
21	6.239	1525	1539	1562	rBV	280004	550361	74.66%	10.217%
22	6.415	1590	1594	1596	rVB	380	263	0.04%	0.005%
23	6.489	1612	1617	1619	rBV2	237	246	0.03%	0.005%
24	6.525	1619	1628	1637	rVB6	3725	6607	0.90%	0.123%
25	6.605	1642	1653	1656	rBV4	1636	2900	0.39%	0.054%
26	6.682	1664	1677	1694	rBV2	119395	235621	31.96%	4.374%
27	6.763	1700	1702	1706	rVB3	452	309	0.04%	0.006%
28	7.187	1825	1834	1836	rBV3	1397	1331	0.18%	0.025%
29	7.264	1854	1858	1863	rBV2	241	216	0.03%	0.004%
30	7.560	1938	1950	1970	rBV	56938	105159	14.27%	1.952%
31	7.695	1988	1992	1994	rBV2	384	310	0.04%	0.006%
32	7.711	1994	1997	2000	rVV2	516	355	0.05%	0.007%
33	7.891	2040	2053	2074	rBV	221931	383893	52.08%	7.127%
34	8.123	2117	2125	2129	rBV2	314	438	0.06%	0.008%
35	8.177	2132	2142	2161	rVV	38741	70880	9.62%	1.316%
36	8.325	2184	2188	2191	rVV	398	348	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059380.D
 Acq On : 20 Jun 2024 15:10
 Operator : MD/SY
 Sample : P2960-14
 Misc : 5.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB51

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\SFAMULM052924WMA.M
 Title : VOC Analysis

37	8.354	2194	2197	2201	rVV2	382	312	0.04%	0.006%
38	8.380	2201	2205	2215	rVB2	328	498	0.07%	0.009%
39	8.547	2253	2257	2265	rBV4	1550	1756	0.24%	0.033%
40	8.640	2273	2286	2318	rBV	131603	302651	41.06%	5.618%
41	8.849	2348	2351	2353	rBV	391	217	0.03%	0.004%
42	8.917	2369	2372	2377	rBV2	449	392	0.05%	0.007%
43	9.068	2413	2419	2425	rBV2	227	340	0.05%	0.006%
44	9.113	2428	2433	2438	rBV2	338	455	0.06%	0.008%
45	9.203	2458	2461	2464	rBV4	1366	1228	0.17%	0.023%
46	9.332	2493	2501	2508	rVV3	1825	2558	0.35%	0.047%
47	9.412	2513	2526	2564	rVV	405903	718136	97.42%	13.331%
48	9.663	2597	2604	2607	rBV6	545	637	0.09%	0.012%
49	9.705	2607	2617	2623	rBV6	1928	3401	0.46%	0.063%
50	9.817	2647	2652	2655	rBV	292	323	0.04%	0.006%
51	9.862	2663	2666	2671	rVB3	632	461	0.06%	0.009%
52	9.955	2692	2695	2700	rVB3	323	254	0.03%	0.005%
53	10.017	2705	2714	2725	rBV5	4459	7829	1.06%	0.145%
54	10.071	2728	2731	2733	rBV3	480	354	0.05%	0.007%
55	10.113	2735	2744	2749	rBV5	2982	4283	0.58%	0.080%
56	10.248	2767	2786	2798	rBV3	13578	25021	3.39%	0.464%
57	10.312	2798	2806	2808	rVV5	2540	3545	0.48%	0.066%
58	10.348	2809	2817	2824	rVV6	9117	19221	2.61%	0.357%
59	10.390	2825	2830	2842	rVV3	10098	15773	2.14%	0.293%
60	10.457	2843	2851	2862	rVB3	2639	4943	0.67%	0.092%
61	10.557	2867	2882	2889	rBV9	8083	18138	2.46%	0.337%
62	10.621	2896	2902	2907	rBV4	8079	10247	1.39%	0.190%
63	10.753	2931	2943	2955	rBV	210506	349549	47.42%	6.489%
64	10.885	2979	2984	2986	rBV4	579	624	0.08%	0.012%
65	10.949	2997	3004	3014	rBV7	3668	6192	0.84%	0.115%
66	11.016	3017	3025	3028	rBV9	3258	4810	0.65%	0.089%
67	11.058	3032	3038	3049	rVB8	10845	18857	2.56%	0.350%
68	11.373	3130	3136	3140	rBV7	2835	4108	0.56%	0.076%
69	11.412	3141	3148	3156	rVV3	17929	26091	3.54%	0.484%
70	11.470	3157	3166	3183	rVB3	15834	33469	4.54%	0.621%
71	11.566	3188	3196	3198	rBV5	2021	2470	0.34%	0.046%
72	11.708	3232	3240	3248	rBV3	10640	15654	2.12%	0.291%
73	11.811	3260	3272	3289	rBV	445403	737165	100.00%	13.685%
74	12.087	3354	3358	3359	rBV3	765	548	0.07%	0.010%
75	12.190	3377	3390	3412	rBV	252110	422068	57.26%	7.835%
76	12.322	3429	3431	3435	rBV4	834	633	0.09%	0.012%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
 Data File : VU059380.D
 Acq On : 20 Jun 2024 15:10
 Operator : MD/SY
 Sample : P2960-14
 Misc : 5.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB51

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\SFAMULM052924WMA.M
 Title : VOC Analysis

77	12.473	3473	3478	3482	rBV5	1139	1128	0.15%	0.021%
78	12.573	3505	3509	3517	rVB4	993	1467	0.20%	0.027%
79	12.608	3517	3520	3527	rBV2	513	610	0.08%	0.011%
80	12.836	3588	3591	3598	rBV2	386	314	0.04%	0.006%
81	12.875	3601	3603	3608	rBV3	343	283	0.04%	0.005%
82	12.930	3613	3620	3623	rBV2	738	882	0.12%	0.016%
83	13.039	3651	3654	3657	rVB4	824	546	0.07%	0.010%
84	13.232	3711	3714	3719	rVB2	336	248	0.03%	0.005%
85	13.354	3749	3752	3757	rBV	229	244	0.03%	0.005%
86	13.521	3801	3804	3807	rVV2	384	234	0.03%	0.004%
87	13.814	3890	3895	3898	rBV	415	431	0.06%	0.008%
88	14.119	3983	3990	3996	rBV2	1014	1698	0.23%	0.032%
89	14.331	4050	4056	4058	rBV2	352	382	0.05%	0.007%
90	14.476	4097	4101	4110	rVB2	418	609	0.08%	0.011%
91	14.592	4132	4137	4139	rBV2	367	364	0.05%	0.007%
92	14.637	4148	4151	4158	rBV3	316	372	0.05%	0.007%
93	15.003	4262	4265	4266	rBV2	367	213	0.03%	0.004%
94	15.241	4336	4339	4344	rBV3	342	469	0.06%	0.009%
95	15.602	4448	4451	4454	rBV2	636	456	0.06%	0.008%
96	15.637	4459	4462	4465	rVV4	459	278	0.04%	0.005%
97	15.749	4495	4497	4500	rVB2	510	237	0.03%	0.004%
98	15.875	4534	4536	4539	rBV2	496	304	0.04%	0.006%
99	15.978	4560	4568	4575	rBV7	1829	2328	0.32%	0.043%
100	16.290	4660	4665	4674	rVB6	2956	3385	0.46%	0.063%

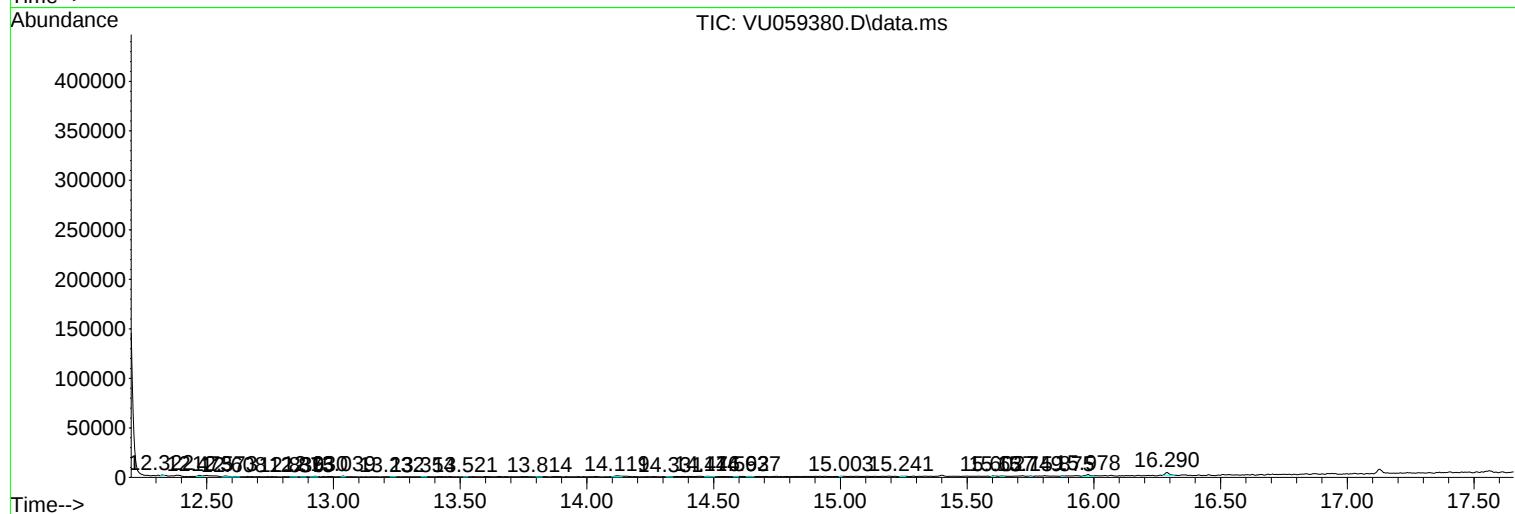
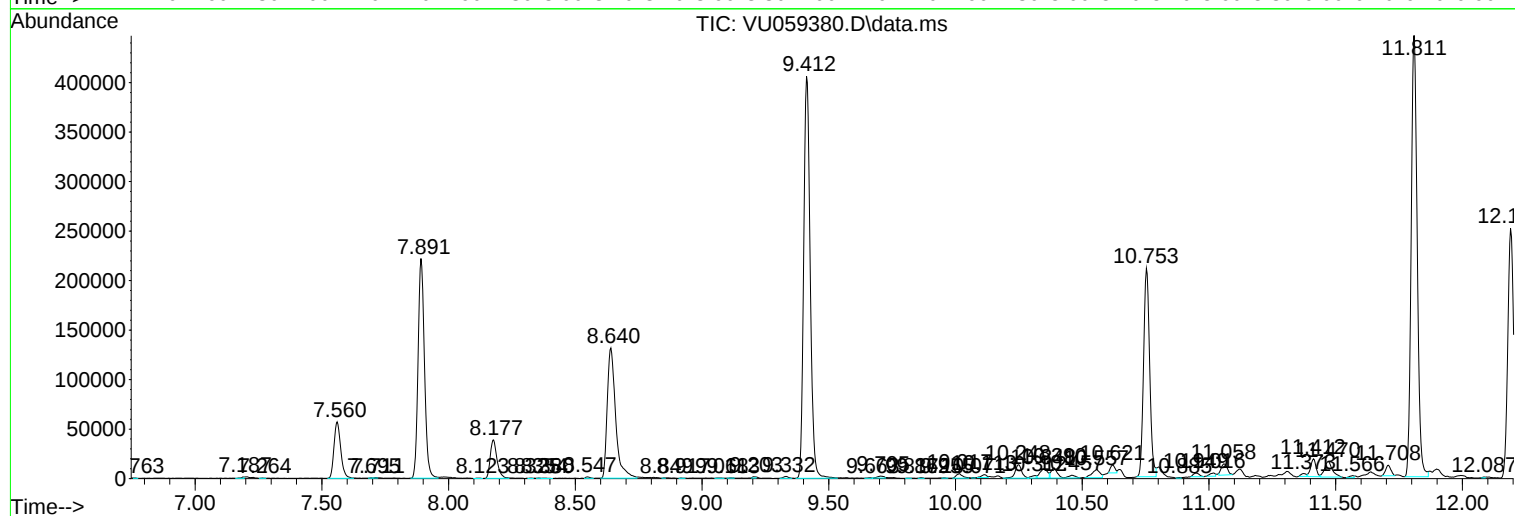
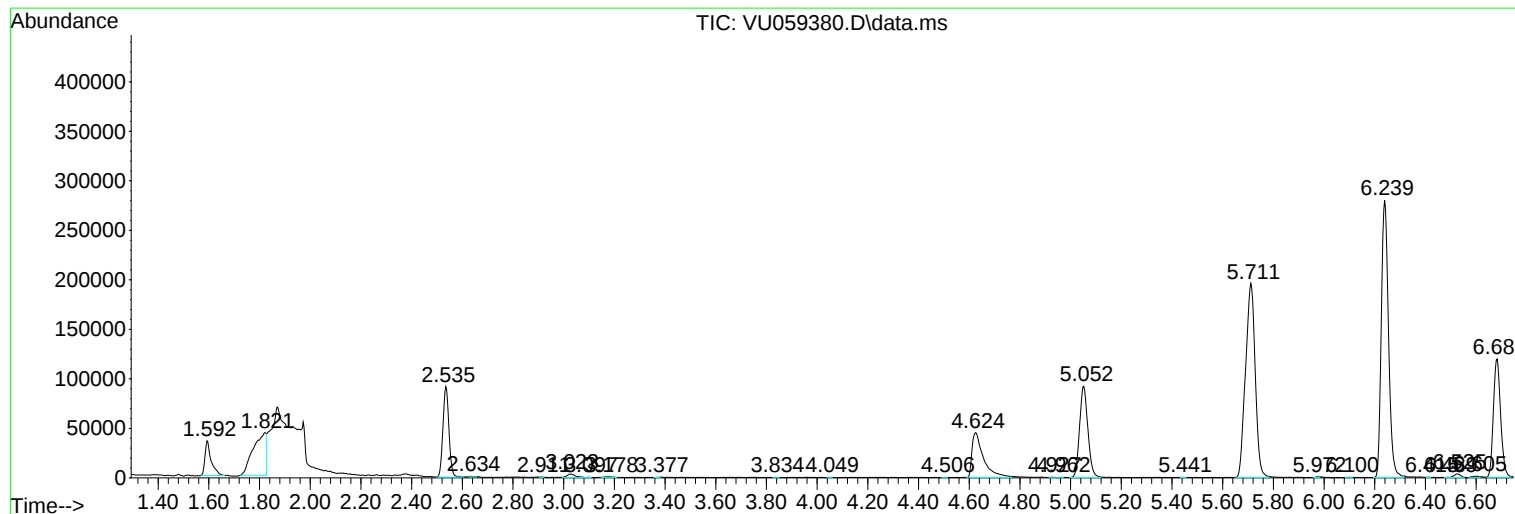
Sum of corrected areas: 5386821

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059380.D
Acq On : 20 Jun 2024 15:10
Operator : MD/SY
Sample : P2960-14
Misc : 5.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB51

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062024\
Data File : VU059380.D
Acq On : 20 Jun 2024 15:10
Operator : MD/SY
Sample : P2960-14
Misc : 5.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB51

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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\VU062024\
Data File : VU059380.D
Acq On : 20 Jun 2024 15:10
Operator : MD/SY
Sample : P2960-14
Misc : 5.95g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB51

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

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