

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
 Data File : VU059067.D
 Acq On : 29 May 2024 21:27
 Operator : MD/SY
 Sample : P2590-11ME
 Misc : 5.43g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHBL7ME

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: VU059067.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	54	59	65	rBV3	2383	2526	0.24%	0.028%
2	1.592	86	94	121	rVB	94945	137357	13.14%	1.512%
3	1.872	136	181	194	rBV	158252	659391	63.09%	7.259%
4	2.541	377	389	410	rVB	196401	320758	30.69%	3.531%
5	2.628	411	416	417	rBV3	788	604	0.06%	0.007%
6	2.669	427	429	433	rVB	394	241	0.02%	0.003%
7	2.756	452	456	459	rBV3	1140	1060	0.10%	0.012%
8	2.869	487	491	494	rBV3	240	194	0.02%	0.002%
9	2.930	507	510	513	rBV2	326	221	0.02%	0.002%
10	3.033	530	542	557	rVB4	4252	8686	0.83%	0.096%
11	3.103	557	564	567	rBV2	184	227	0.02%	0.002%
12	3.171	572	585	602	rBV	8827	21752	2.08%	0.239%
13	3.264	612	614	618	rBV2	335	208	0.02%	0.002%
14	3.586	710	714	717	rBV	260	246	0.02%	0.003%
15	3.682	741	744	748	rVB3	557	306	0.03%	0.003%
16	3.827	784	789	796	rVB2	262	341	0.03%	0.004%
17	3.865	796	801	803	rBV	265	251	0.02%	0.003%
18	3.910	811	815	817	rBV	318	273	0.03%	0.003%
19	4.245	917	919	928	rBV2	287	293	0.03%	0.003%
20	4.367	951	957	959	rBV2	215	212	0.02%	0.002%
21	4.615	1023	1034	1084	rBV	108450	321852	30.79%	3.543%
22	4.849	1103	1107	1110	rBV4	396	371	0.04%	0.004%
23	5.052	1154	1170	1199	rBV	186362	423424	40.51%	4.662%
24	5.254	1229	1233	1236	rBV2	265	265	0.03%	0.003%
25	5.312	1242	1251	1254	rBV2	208	288	0.03%	0.003%
26	5.341	1256	1260	1265	rBV2	327	392	0.04%	0.004%
27	5.441	1286	1291	1295	rVB2	284	348	0.03%	0.004%
28	5.627	1347	1349	1355	rVB	289	205	0.02%	0.002%
29	5.711	1355	1375	1399	rBV2	389703	1045234	100.00%	11.507%
30	5.930	1441	1443	1449	rVB3	210	189	0.02%	0.002%
31	5.975	1449	1457	1464	rBV6	1726	3551	0.34%	0.039%
32	6.238	1526	1539	1560	rBV	349621	675411	64.62%	7.436%
33	6.389	1583	1586	1587	rBV	472	277	0.03%	0.003%
34	6.528	1617	1629	1641	rVB10	8090	16484	1.58%	0.181%
35	6.595	1641	1650	1663	rBV5	2566	5639	0.54%	0.062%
36	6.682	1663	1677	1697	rBV	247283	491252	47.00%	5.408%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
 Data File : VU059067.D
 Acq On : 29 May 2024 21:27
 Operator : MD/SY
 Sample : P2590-11ME
 Misc : 5.43g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHBL7ME

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	6.782	1705	1708	1712	rVB3	873	530	0.05%	0.006%
38	6.807	1712	1716	1720	rVB2	660	524	0.05%	0.006%
39	6.914	1743	1749	1754	rBV	277	372	0.04%	0.004%
40	7.110	1807	1810	1817	rVB2	226	204	0.02%	0.002%
41	7.193	1830	1836	1837	rBV2	817	564	0.05%	0.006%
42	7.222	1843	1845	1851	rVB4	808	741	0.07%	0.008%
43	7.560	1938	1950	1970	rBV	120824	221966	21.24%	2.444%
44	7.640	1973	1975	1983	rVB3	432	363	0.03%	0.004%
45	7.705	1989	1995	1996	rBV2	566	502	0.05%	0.006%
46	7.775	2014	2017	2019	rBV	348	256	0.02%	0.003%
47	7.891	2038	2053	2076	rBV	449828	783238	74.93%	8.623%
48	8.042	2098	2100	2106	rVB4	639	430	0.04%	0.005%
49	8.094	2111	2116	2119	rBV4	374	364	0.03%	0.004%
50	8.174	2130	2141	2160	rBV2	82543	151623	14.51%	1.669%
51	8.241	2160	2162	2166	rVB3	368	244	0.02%	0.003%
52	8.354	2194	2197	2201	rBV2	452	371	0.04%	0.004%
53	8.460	2226	2230	2235	rVV3	503	521	0.05%	0.006%
54	8.637	2270	2285	2321	rBV2	290520	673039	64.39%	7.410%
55	8.917	2370	2372	2376	rVB3	570	360	0.03%	0.004%
56	8.939	2376	2379	2382	rBV3	388	239	0.02%	0.003%
57	8.955	2382	2384	2388	rVB2	409	308	0.03%	0.003%
58	9.000	2395	2398	2401	rBV	341	249	0.02%	0.003%
59	9.348	2499	2506	2509	rVB	330	385	0.04%	0.004%
60	9.412	2509	2526	2548	rBV	503083	881242	84.31%	9.702%
61	9.695	2609	2614	2630	rVB3	1224	2656	0.25%	0.029%
62	9.759	2630	2634	2635	rBV2	322	219	0.02%	0.002%
63	9.875	2664	2670	2672	rBV	191	227	0.02%	0.002%
64	9.926	2683	2686	2689	rBV2	303	210	0.02%	0.002%
65	9.968	2694	2699	2705	rVV	171	226	0.02%	0.002%
66	10.135	2748	2751	2754	rBV2	444	262	0.03%	0.003%
67	10.627	2899	2904	2907	rBV2	210	235	0.02%	0.003%
68	10.753	2929	2943	2965	rBV	397680	653129	62.49%	7.190%
69	11.058	3032	3038	3040	rBV2	257	237	0.02%	0.003%
70	11.717	3241	3243	3249	rVV2	236	203	0.02%	0.002%
71	11.765	3254	3258	3259	rBV2	276	196	0.02%	0.002%
72	11.807	3259	3271	3290	rBV	500600	824487	78.88%	9.077%
73	12.109	3362	3365	3371	rBV2	307	322	0.03%	0.004%
74	12.190	3377	3390	3412	rBV	442228	734031	70.23%	8.081%
75	12.335	3433	3435	3439	rVB2	421	252	0.02%	0.003%
76	12.762	3564	3568	3570	rBV2	407	376	0.04%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
 Data File : VU059067.D
 Acq On : 29 May 2024 21:27
 Operator : MD/SY
 Sample : P2590-11ME
 Misc : 5.43g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHBL7ME

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	12.823	3582	3587	3591	rBV	264	251	0.02%	0.003%
78	12.878	3601	3604	3608	rVB	363	207	0.02%	0.002%
79	13.187	3697	3700	3702	rBV	274	190	0.02%	0.002%
80	13.270	3723	3726	3730	rVB2	358	253	0.02%	0.003%
81	13.428	3773	3775	3776	rBV2	451	222	0.02%	0.002%
82	13.746	3871	3874	3876	rBV2	278	207	0.02%	0.002%
83	13.910	3922	3925	3928	rBV	312	191	0.02%	0.002%
84	14.090	3977	3981	3983	rBV2	319	251	0.02%	0.003%
85	14.351	4059	4062	4065	rBV	374	285	0.03%	0.003%
86	14.405	4075	4079	4083	rVB2	357	318	0.03%	0.004%
87	14.453	4091	4094	4095	rBV2	400	235	0.02%	0.003%
88	14.495	4102	4107	4116	rVB2	467	574	0.05%	0.006%
89	14.543	4118	4122	4126	rBV3	406	350	0.03%	0.004%
90	14.743	4181	4184	4187	rBV2	353	294	0.03%	0.003%
91	15.396	4384	4387	4389	rBV	460	289	0.03%	0.003%
92	15.566	4437	4440	4444	rBV2	338	243	0.02%	0.003%
93	15.659	4467	4469	4472	rBV3	342	249	0.02%	0.003%
94	15.987	4569	4571	4574	rBV3	459	207	0.02%	0.002%
95	16.235	4645	4648	4649	rBV	630	342	0.03%	0.004%
96	16.357	4683	4686	4689	rBV3	632	410	0.04%	0.005%
97	16.463	4717	4719	4723	rVB2	622	426	0.04%	0.005%
98	16.543	4742	4744	4745	rBV2	470	192	0.02%	0.002%
99	16.688	4787	4789	4793	rBV3	806	469	0.04%	0.005%
100	16.939	4865	4867	4869	rBV3	960	496	0.05%	0.005%

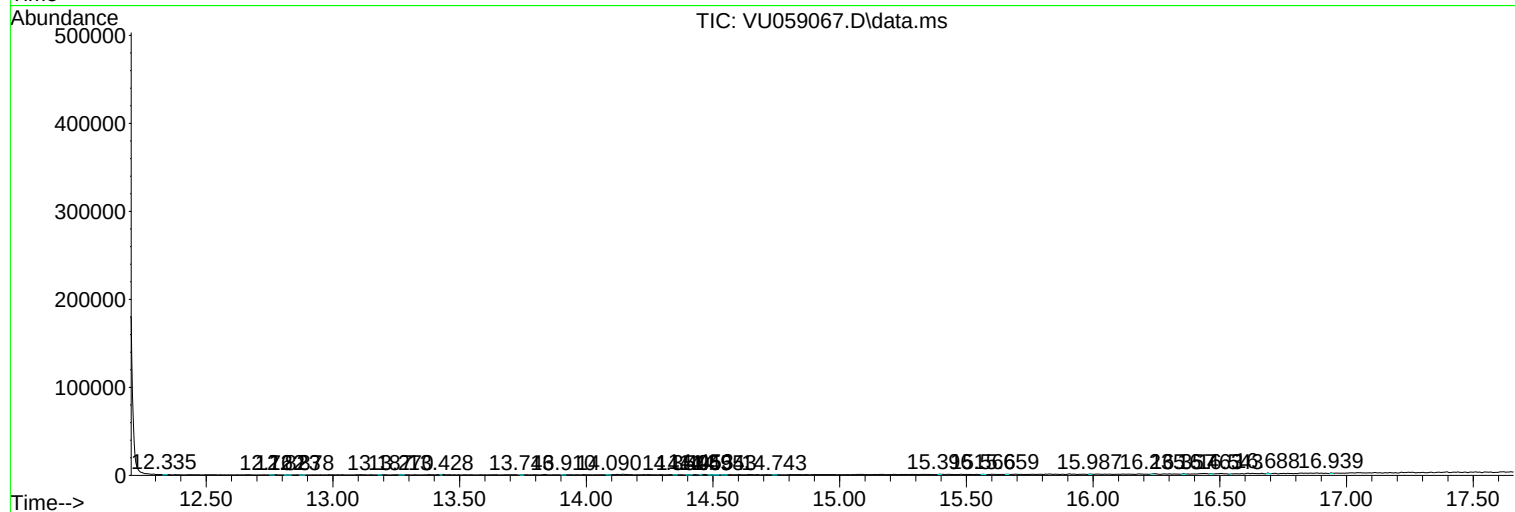
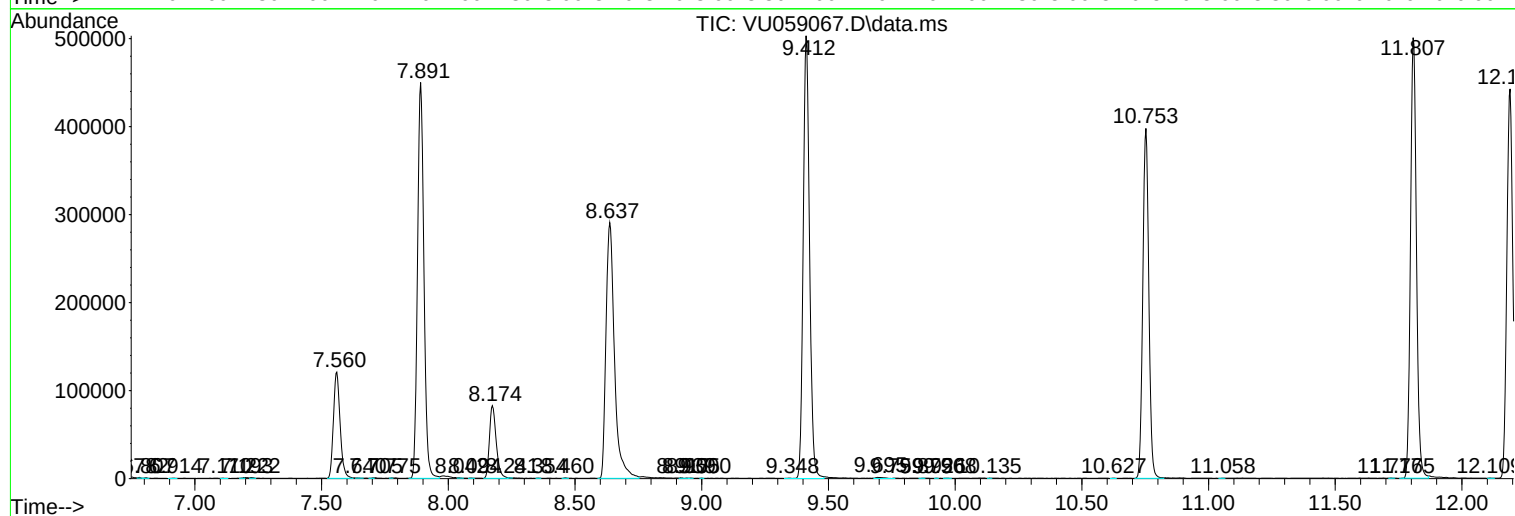
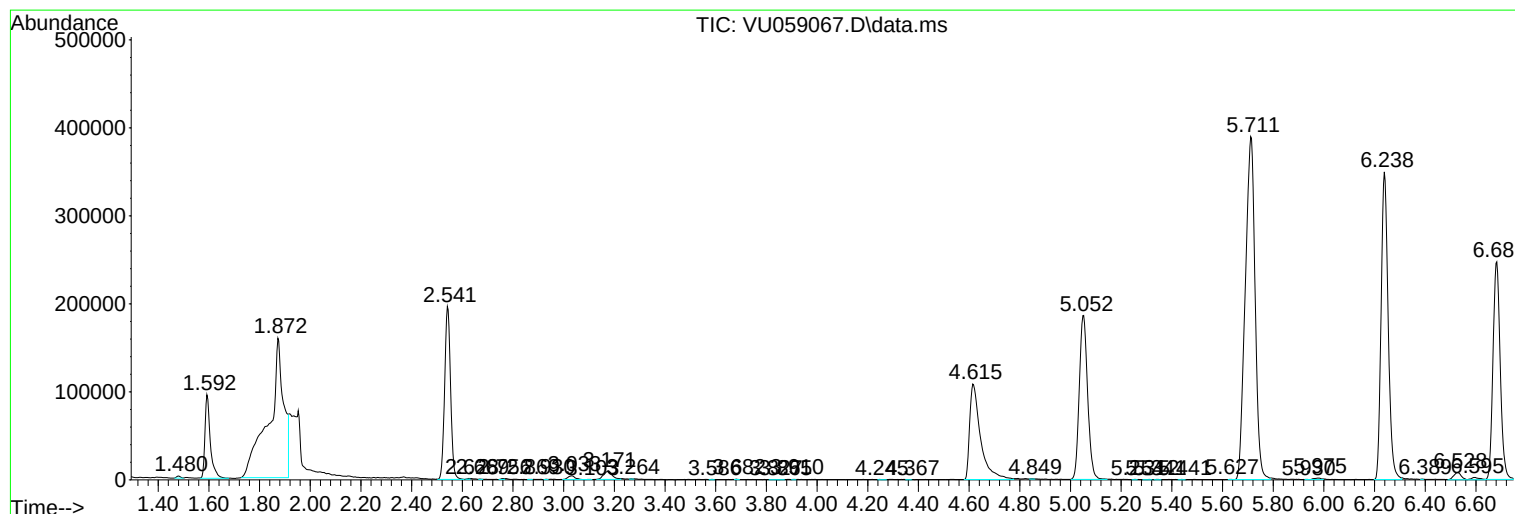
Sum of corrected areas: 9083383

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
Data File : VU059067.D
Acq On : 29 May 2024 21:27
Operator : MD/SY
Sample : P2590-11ME
Misc : 5.43g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHBL7ME

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\VU052924\
Data File : VU059067.D
Acq On : 29 May 2024 21:27
Operator : MD/SY
Sample : P2590-11ME
Misc : 5.43g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHBL7ME

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\VU052924\
Data File : VU059067.D
Acq On : 29 May 2024 21:27
Operator : MD/SY
Sample : P2590-11ME
Misc : 5.43g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHBL7ME

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
------------------	----	---------	-------	----------	---	----	------	------