

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059251.D
 Acq On : 14 Jun 2024 16:34
 Operator : MD/SY
 Sample : P2798-03ME
 Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB14ME

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: VU059251.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.483	55	60	65	rVB3	1741	1787	0.23%	0.025%
2	1.592	87	94	114	rVB	38305	67596	8.57%	0.940%
3	1.837	136	170	172	rBV4	54565	224537	28.45%	3.122%
4	2.409	344	348	351	rBV4	1306	1133	0.14%	0.016%
5	2.541	377	389	404	rBV	108030	176100	22.32%	2.448%
6	2.615	407	412	413	rBV3	518	375	0.05%	0.005%
7	2.763	453	458	461	rBV	746	711	0.09%	0.010%
8	2.914	503	505	510	rVB2	321	257	0.03%	0.004%
9	2.943	511	514	519	rBV3	201	231	0.03%	0.003%
10	3.030	531	541	555	rBV3	4405	9392	1.19%	0.131%
11	3.171	572	585	602	rBV	6686	17008	2.16%	0.236%
12	3.338	631	637	640	rBV2	497	521	0.07%	0.007%
13	3.586	711	714	718	rBV2	243	250	0.03%	0.003%
14	3.605	718	720	726	rVB2	231	242	0.03%	0.003%
15	3.686	742	745	748	rBV	364	212	0.03%	0.003%
16	3.821	784	787	793	rVV	249	289	0.04%	0.004%
17	3.878	799	805	809	rVB2	213	225	0.03%	0.003%
18	4.052	856	859	863	rBV2	215	225	0.03%	0.003%
19	4.235	912	916	921	rBV2	170	206	0.03%	0.003%
20	4.293	931	934	939	rVB2	284	272	0.03%	0.004%
21	4.618	1024	1035	1071	rBV	128737	425813	53.96%	5.920%
22	4.936	1130	1134	1137	rBV3	357	319	0.04%	0.004%
23	5.052	1154	1170	1193	rBV	161484	357841	45.35%	4.975%
24	5.161	1201	1204	1208	rBV3	300	273	0.03%	0.004%
25	5.248	1228	1231	1234	rVB3	300	186	0.02%	0.003%
26	5.274	1234	1239	1243	rBV3	407	326	0.04%	0.005%
27	5.711	1356	1375	1404	rVV2	285439	788008	99.86%	10.956%
28	5.933	1441	1444	1447	rVB2	357	240	0.03%	0.003%
29	5.975	1447	1457	1459	rBV4	1400	1574	0.20%	0.022%
30	6.055	1480	1482	1486	rVB2	270	193	0.02%	0.003%
31	6.094	1490	1494	1498	rVB	261	228	0.03%	0.003%
32	6.139	1503	1508	1513	rBV2	197	194	0.02%	0.003%
33	6.242	1522	1540	1564	rBV	238188	462098	58.56%	6.425%
34	6.528	1618	1629	1643	rBV6	9098	18471	2.34%	0.257%
35	6.599	1643	1651	1658	rBV6	1407	2574	0.33%	0.036%
36	6.682	1663	1677	1700	rBV	203134	409413	51.88%	5.692%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059251.D
 Acq On : 14 Jun 2024 16:34
 Operator : MD/SY
 Sample : P2798-03ME
 Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB14ME

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	6.779	1705	1707	1710	rBV2	305	195	0.02%	0.003%
38	7.193	1829	1836	1838	rBV4	1633	1951	0.25%	0.027%
39	7.271	1853	1860	1862	rBV2	229	215	0.03%	0.003%
40	7.328	1874	1878	1881	rBV	308	204	0.03%	0.003%
41	7.428	1907	1909	1914	rVV2	299	194	0.02%	0.003%
42	7.560	1937	1950	1971	rBV2	94763	175102	22.19%	2.434%
43	7.711	1989	1997	2000	rBV4	1028	1292	0.16%	0.018%
44	7.891	2040	2053	2075	rBV	289081	511465	64.81%	7.111%
45	8.052	2100	2103	2107	rVB2	351	297	0.04%	0.004%
46	8.078	2107	2111	2113	rBV	347	227	0.03%	0.003%
47	8.177	2130	2142	2163	rBV	64962	118286	14.99%	1.645%
48	8.467	2227	2232	2237	rBV2	200	252	0.03%	0.004%
49	8.550	2246	2258	2269	rVB6	6319	11157	1.41%	0.155%
50	8.637	2272	2285	2316	rBV	353040	789133	100.00%	10.971%
51	8.856	2349	2353	2355	rBV3	472	399	0.05%	0.006%
52	8.910	2367	2370	2372	rBV2	324	247	0.03%	0.003%
53	8.994	2390	2396	2402	rVB2	460	468	0.06%	0.007%
54	9.062	2413	2417	2419	rBV	319	250	0.03%	0.003%
55	9.190	2450	2457	2459	rBV	377	452	0.06%	0.006%
56	9.328	2497	2500	2504	rVB2	251	208	0.03%	0.003%
57	9.415	2514	2527	2554	rBV	345961	608675	77.13%	8.462%
58	9.698	2608	2615	2620	rBV3	1338	1653	0.21%	0.023%
59	10.110	2737	2743	2747	rBV3	468	536	0.07%	0.007%
60	10.139	2750	2752	2758	rVB2	408	369	0.05%	0.005%
61	10.225	2773	2779	2782	rBV2	180	188	0.02%	0.003%
62	10.351	2815	2818	2827	rBV2	217	273	0.03%	0.004%
63	10.418	2834	2839	2843	rBV2	175	212	0.03%	0.003%
64	10.483	2853	2859	2861	rBV3	326	331	0.04%	0.005%
65	10.753	2928	2943	2965	rBV	453291	750436	95.10%	10.433%
66	10.888	2982	2985	2988	rBV	417	296	0.04%	0.004%
67	11.103	3047	3052	3053	rBV	272	222	0.03%	0.003%
68	11.203	3080	3083	3089	rVB	230	192	0.02%	0.003%
69	11.389	3138	3141	3145	rVB2	242	189	0.02%	0.003%
70	11.483	3165	3170	3174	rBV2	554	481	0.06%	0.007%
71	11.505	3174	3177	3183	rVB2	222	236	0.03%	0.003%
72	11.640	3213	3219	3221	rBV	266	271	0.03%	0.004%
73	11.743	3247	3251	3252	rBV2	733	403	0.05%	0.006%
74	11.811	3259	3272	3296	rBV	341611	566019	71.73%	7.869%
75	11.968	3318	3321	3325	rVB2	415	367	0.05%	0.005%
76	12.077	3352	3355	3358	rBV	240	188	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
 Data File : VU059251.D
 Acq On : 14 Jun 2024 16:34
 Operator : MD/SY
 Sample : P2798-03ME
 Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB14ME

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	12.190	3377	3390	3412	rBV	398461	671559	85.10%	9.337%
78	12.335	3432	3435	3437	rBV2	470	267	0.03%	0.004%
79	12.492	3481	3484	3489	rBV	314	208	0.03%	0.003%
80	12.772	3565	3571	3575	rBV2	626	772	0.10%	0.011%
81	13.171	3692	3695	3698	rBV	256	188	0.02%	0.003%
82	13.463	3784	3786	3792	rVB	328	287	0.04%	0.004%
83	13.682	3850	3854	3857	rBV2	548	399	0.05%	0.006%
84	13.778	3881	3884	3887	rVB3	490	309	0.04%	0.004%
85	13.827	3895	3899	3901	rBV2	266	223	0.03%	0.003%
86	13.897	3918	3921	3926	rVB2	432	364	0.05%	0.005%
87	14.007	3948	3955	3960	rBV3	480	563	0.07%	0.008%
88	14.077	3974	3977	3980	rVB2	347	247	0.03%	0.003%
89	14.122	3987	3991	3996	rBV2	474	608	0.08%	0.008%
90	14.351	4058	4062	4066	rBV2	432	400	0.05%	0.006%
91	14.473	4096	4100	4105	rVV2	330	358	0.05%	0.005%
92	14.650	4152	4155	4158	rBV3	310	262	0.03%	0.004%
93	14.746	4183	4185	4188	rVB2	479	271	0.03%	0.004%
94	14.765	4188	4191	4195	rBV2	359	374	0.05%	0.005%
95	14.814	4203	4206	4209	rBV	486	428	0.05%	0.006%
96	15.225	4331	4334	4336	rBV2	377	255	0.03%	0.004%
97	15.309	4357	4360	4361	rBV	399	261	0.03%	0.004%
98	15.900	4542	4544	4547	rBV	807	467	0.06%	0.006%
99	15.946	4556	4558	4561	rBV3	443	219	0.03%	0.003%
100	16.023	4580	4582	4586	rBV2	529	487	0.06%	0.007%

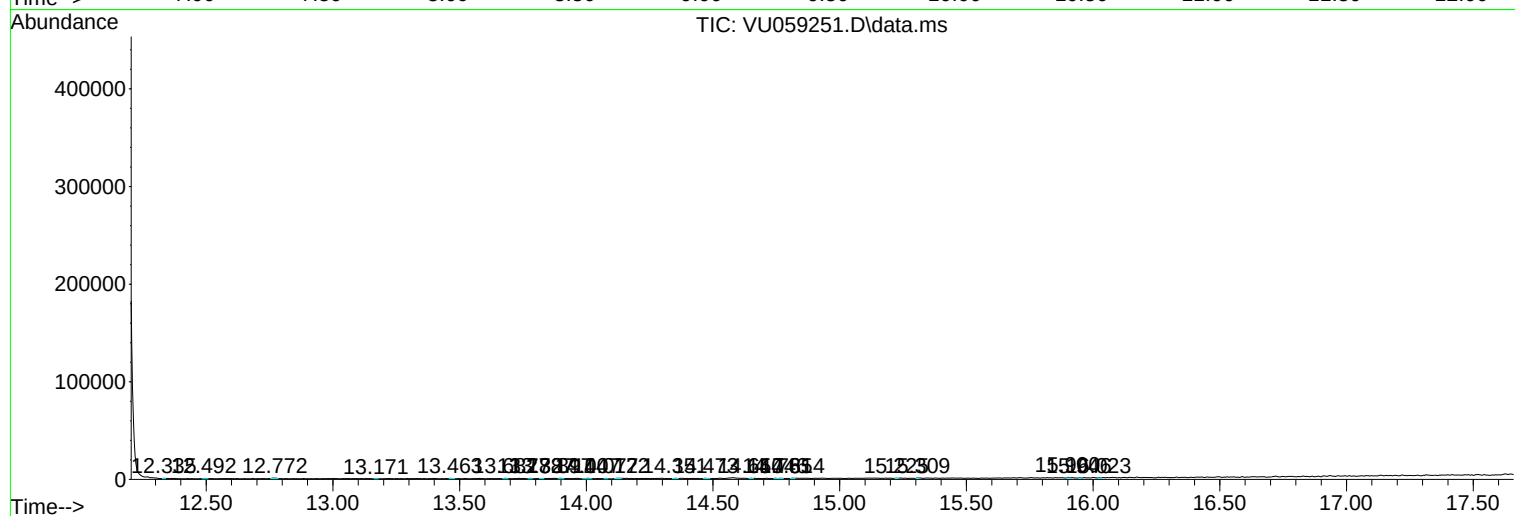
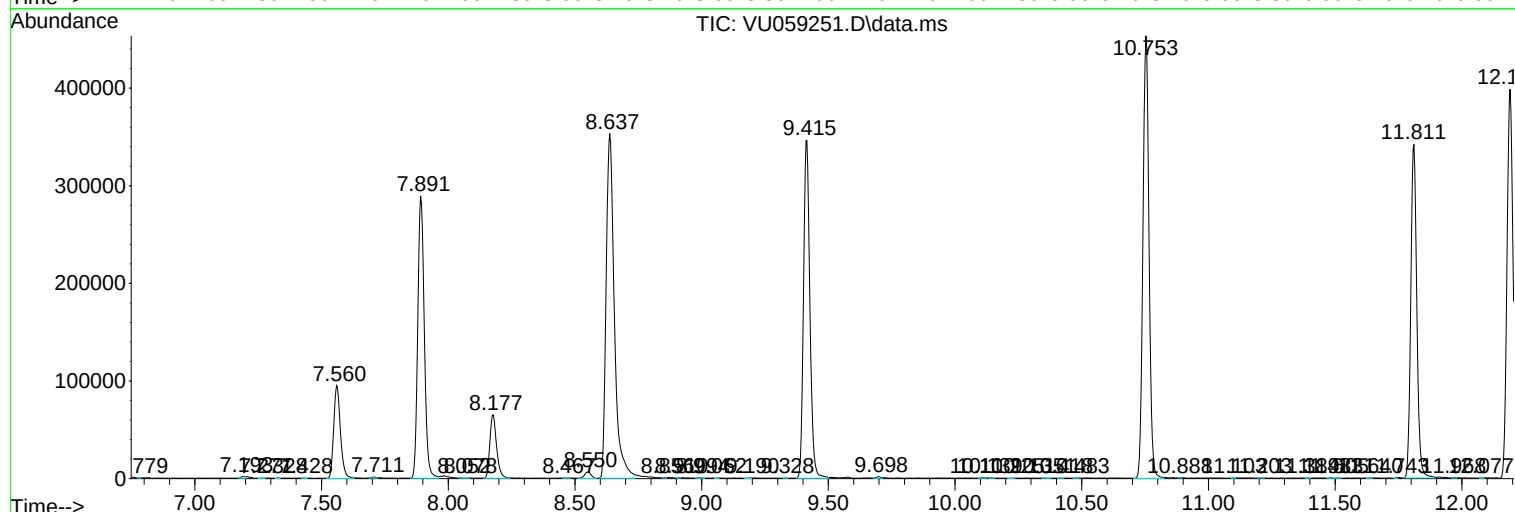
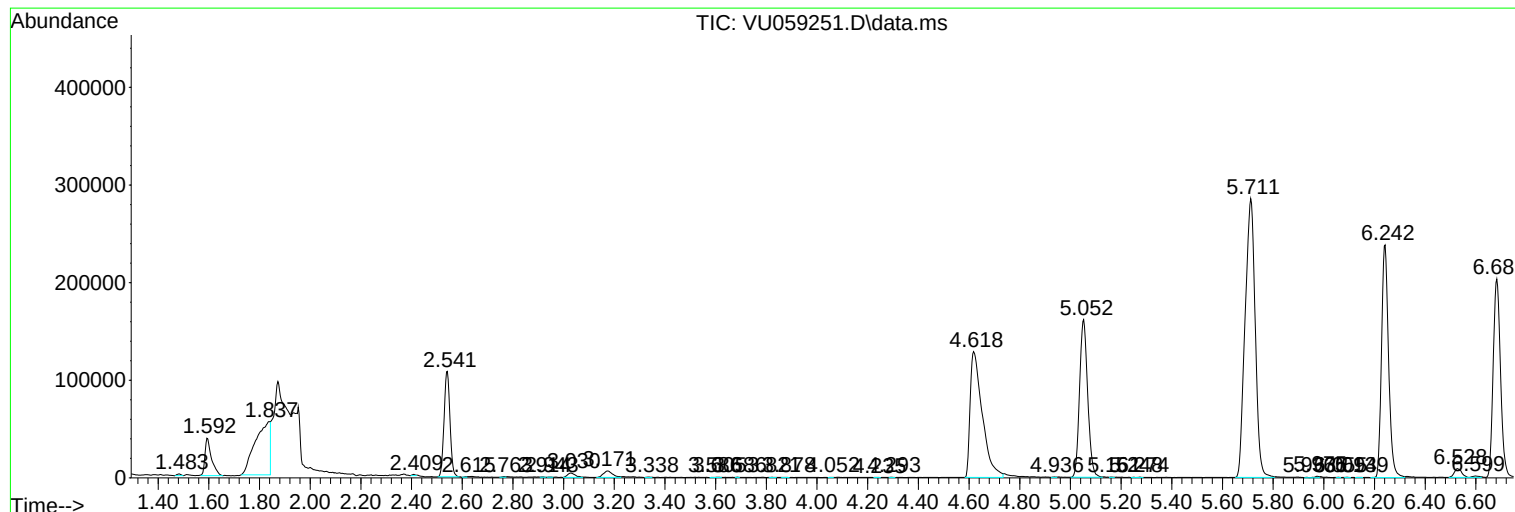
Sum of corrected areas: 7192627

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061424\
Data File : VU059251.D
Acq On : 14 Jun 2024 16:34
Operator : MD/SY
Sample : P2798-03ME
Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB14ME

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\VU061424\
Data File : VU059251.D
Acq On : 14 Jun 2024 16:34
Operator : MD/SY
Sample : P2798-03ME
Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB14ME

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\VU061424\
Data File : VU059251.D
Acq On : 14 Jun 2024 16:34
Operator : MD/SY
Sample : P2798-03ME
Misc : 5.39g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB14ME

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