

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059301.D
 Acq On : 18 Jun 2024 10:57
 Operator : MD/SY
 Sample : P2850-08ME
 Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB09ME

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: VU059301.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	55	59	66	rBV2	1413	1326	0.17%	0.020%
2	1.592	86	94	120	rVB	53531	98188	12.62%	1.505%
3	1.872	137	181	194	rBV2	81684	426808	54.84%	6.542%
4	2.367	331	335	340	rVB5	1846	1935	0.25%	0.030%
5	2.538	375	388	405	rBV	148667	245333	31.52%	3.760%
6	2.618	411	413	416	rBV2	450	351	0.05%	0.005%
7	2.637	416	419	422	rVV3	611	562	0.07%	0.009%
8	2.798	465	469	472	rBV3	451	336	0.04%	0.005%
9	3.026	531	540	555	rBV2	5324	10271	1.32%	0.157%
10	3.197	590	593	598	rVB2	347	307	0.04%	0.005%
11	3.361	642	644	647	rBV2	332	254	0.03%	0.004%
12	3.422	658	663	666	rBV2	270	322	0.04%	0.005%
13	3.676	735	742	748	rBV	303	433	0.06%	0.007%
14	4.129	880	883	891	rVB2	272	352	0.05%	0.005%
15	4.181	891	899	904	rBV2	274	418	0.05%	0.006%
16	4.280	926	930	935	rVB2	265	262	0.03%	0.004%
17	4.364	952	956	962	rBV	312	397	0.05%	0.006%
18	4.406	967	969	975	rVB2	272	258	0.03%	0.004%
19	4.435	975	978	983	rVB	323	276	0.04%	0.004%
20	4.560	1009	1017	1022	rBV2	323	528	0.07%	0.008%
21	4.624	1026	1037	1080	rBV	66444	226482	29.10%	3.471%
22	5.052	1153	1170	1201	rBV	137936	308202	39.60%	4.724%
23	5.329	1249	1256	1259	rBV2	248	263	0.03%	0.004%
24	5.711	1356	1375	1403	rBV2	291867	778247	100.00%	11.928%
25	5.865	1420	1423	1428	rVB2	327	276	0.04%	0.004%
26	5.978	1448	1458	1463	rBV4	969	1540	0.20%	0.024%
27	6.126	1501	1504	1507	rBV	322	255	0.03%	0.004%
28	6.242	1526	1540	1565	rBV	261320	508170	65.30%	7.789%
29	6.390	1581	1586	1587	rBV2	300	259	0.03%	0.004%
30	6.399	1587	1589	1594	rVB2	504	340	0.04%	0.005%
31	6.441	1597	1602	1606	rVB	398	314	0.04%	0.005%
32	6.480	1611	1614	1620	rVB2	246	266	0.03%	0.004%
33	6.528	1620	1629	1643	rBV7	6660	12853	1.65%	0.197%
34	6.592	1643	1649	1651	rBV2	969	996	0.13%	0.015%
35	6.682	1664	1677	1696	rBV	176008	345609	44.41%	5.297%
36	6.914	1746	1749	1756	rVB2	353	416	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059301.D
 Acq On : 18 Jun 2024 10:57
 Operator : MD/SY
 Sample : P2850-08ME
 Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB09ME

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	6.988	1766	1772	1775	rBV2	237	308	0.04%	0.005%
38	7.132	1812	1817	1824	rVB2	320	428	0.05%	0.007%
39	7.193	1829	1836	1837	rBV3	1671	1652	0.21%	0.025%
40	7.463	1914	1920	1925	rBV2	247	303	0.04%	0.005%
41	7.499	1925	1931	1936	rVB2	202	273	0.04%	0.004%
42	7.560	1936	1950	1973	rBV	85621	156081	20.06%	2.392%
43	7.708	1985	1996	2001	rBV3	1166	1931	0.25%	0.030%
44	7.730	2001	2003	2009	rVB4	478	376	0.05%	0.006%
45	7.804	2020	2026	2028	rBV3	313	343	0.04%	0.005%
46	7.891	2040	2053	2074	rBV	338925	593602	76.27%	9.098%
47	8.071	2106	2109	2112	rBV2	362	341	0.04%	0.005%
48	8.107	2118	2120	2125	rVB2	370	255	0.03%	0.004%
49	8.177	2130	2142	2164	rVB	55499	103138	13.25%	1.581%
50	8.422	2214	2218	2223	rBV2	352	397	0.05%	0.006%
51	8.550	2245	2258	2268	rBV3	6679	10641	1.37%	0.163%
52	8.637	2273	2285	2318	rBV	171025	407819	52.40%	6.251%
53	8.801	2332	2336	2340	rBV3	437	457	0.06%	0.007%
54	9.078	2418	2422	2425	rVB2	311	272	0.03%	0.004%
55	9.103	2425	2430	2433	rBV2	252	264	0.03%	0.004%
56	9.415	2515	2527	2554	rBV	371764	655748	84.26%	10.051%
57	9.537	2563	2565	2570	rBV3	264	251	0.03%	0.004%
58	9.573	2573	2576	2582	rVB3	697	626	0.08%	0.010%
59	9.701	2608	2616	2629	rVB4	1261	2854	0.37%	0.044%
60	9.788	2636	2643	2646	rBV2	227	300	0.04%	0.005%
61	9.859	2661	2665	2668	rBV	332	276	0.04%	0.004%
62	9.933	2683	2688	2694	rVB2	390	553	0.07%	0.008%
63	9.987	2697	2705	2709	rBV2	232	324	0.04%	0.005%
64	10.100	2735	2740	2742	rBV2	447	366	0.05%	0.006%
65	10.142	2749	2753	2759	rBV3	502	698	0.09%	0.011%
66	10.200	2766	2771	2777	rBV	400	568	0.07%	0.009%
67	10.251	2783	2787	2793	rVB2	251	366	0.05%	0.006%
68	10.322	2806	2809	2813	rVB2	378	280	0.04%	0.004%
69	10.569	2877	2886	2891	rVB2	368	570	0.07%	0.009%
70	10.598	2891	2895	2899	rBV2	259	252	0.03%	0.004%
71	10.753	2930	2943	2963	rBV	271722	457665	58.81%	7.015%
72	10.891	2981	2986	2990	rBV2	502	404	0.05%	0.006%
73	10.942	2997	3002	3005	rBV2	256	264	0.03%	0.004%
74	10.978	3008	3013	3018	rVV2	224	291	0.04%	0.004%
75	11.039	3028	3032	3035	rBV2	271	272	0.03%	0.004%
76	11.213	3082	3086	3088	rBV	332	296	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059301.D
 Acq On : 18 Jun 2024 10:57
 Operator : MD/SY
 Sample : P2850-08ME
 Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB09ME

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	11.479	3165	3169	3172	rVV3	259	265	0.03%	0.004%
78	11.634	3214	3217	3223	rVB	291	310	0.04%	0.005%
79	11.749	3245	3253	3260	rBV3	923	1275	0.16%	0.020%
80	11.811	3260	3272	3288	rBV	370177	596458	76.64%	9.142%
81	12.190	3378	3390	3421	rBV	329560	541082	69.53%	8.293%
82	12.299	3422	3424	3428	rVB3	780	394	0.05%	0.006%
83	12.380	3445	3449	3457	rVB2	474	640	0.08%	0.010%
84	12.692	3544	3546	3552	rBV2	277	257	0.03%	0.004%
85	12.769	3566	3570	3574	rVB	833	786	0.10%	0.012%
86	12.897	3602	3610	3614	rBV2	323	440	0.06%	0.007%
87	13.245	3714	3718	3722	rBV4	503	438	0.06%	0.007%
88	13.643	3837	3842	3846	rBV	351	431	0.06%	0.007%
89	13.682	3851	3854	3860	rVV2	282	307	0.04%	0.005%
90	13.782	3881	3885	3887	rBV2	290	274	0.04%	0.004%
91	13.833	3899	3901	3905	rVB2	480	329	0.04%	0.005%
92	13.859	3905	3909	3915	rBV3	524	625	0.08%	0.010%
93	13.987	3946	3949	3956	rBV2	396	480	0.06%	0.007%
94	14.171	4004	4006	4011	rBV3	389	251	0.03%	0.004%
95	14.328	4051	4055	4056	rBV2	367	275	0.04%	0.004%
96	14.573	4124	4131	4142	rVB2	1067	1738	0.22%	0.027%
97	15.071	4282	4286	4293	rVB2	519	647	0.08%	0.010%
98	15.711	4483	4485	4488	rBV2	464	297	0.04%	0.005%
99	16.109	4606	4609	4611	rBV2	633	464	0.06%	0.007%
100	16.244	4648	4651	4653	rBV	598	416	0.05%	0.006%

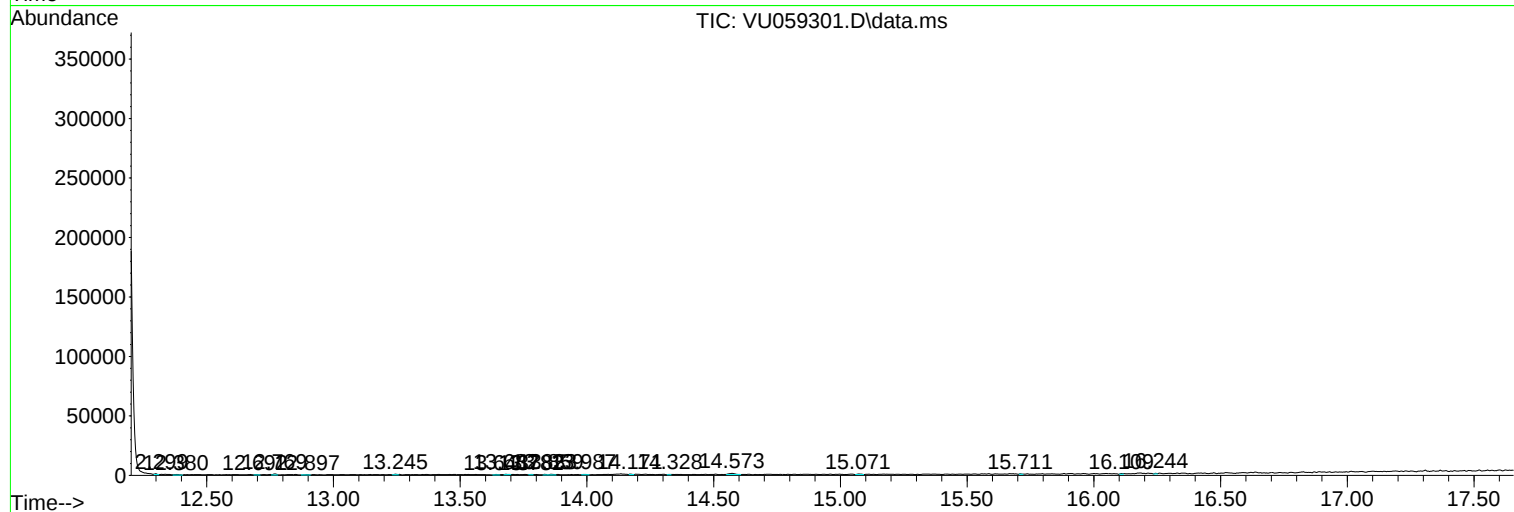
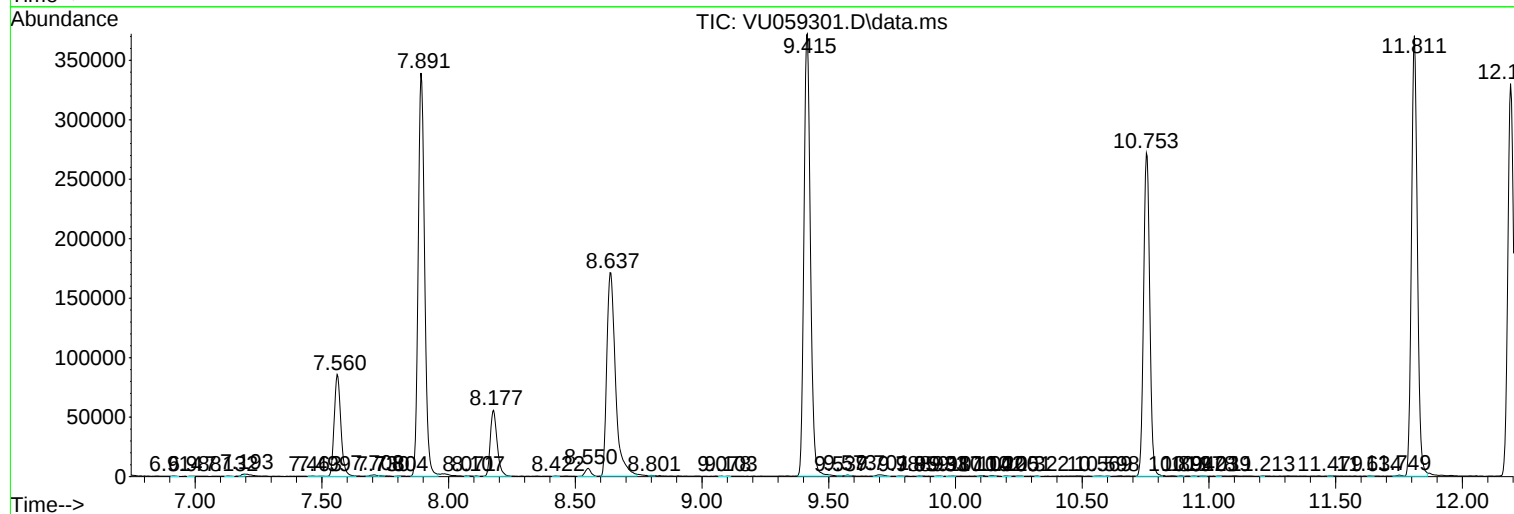
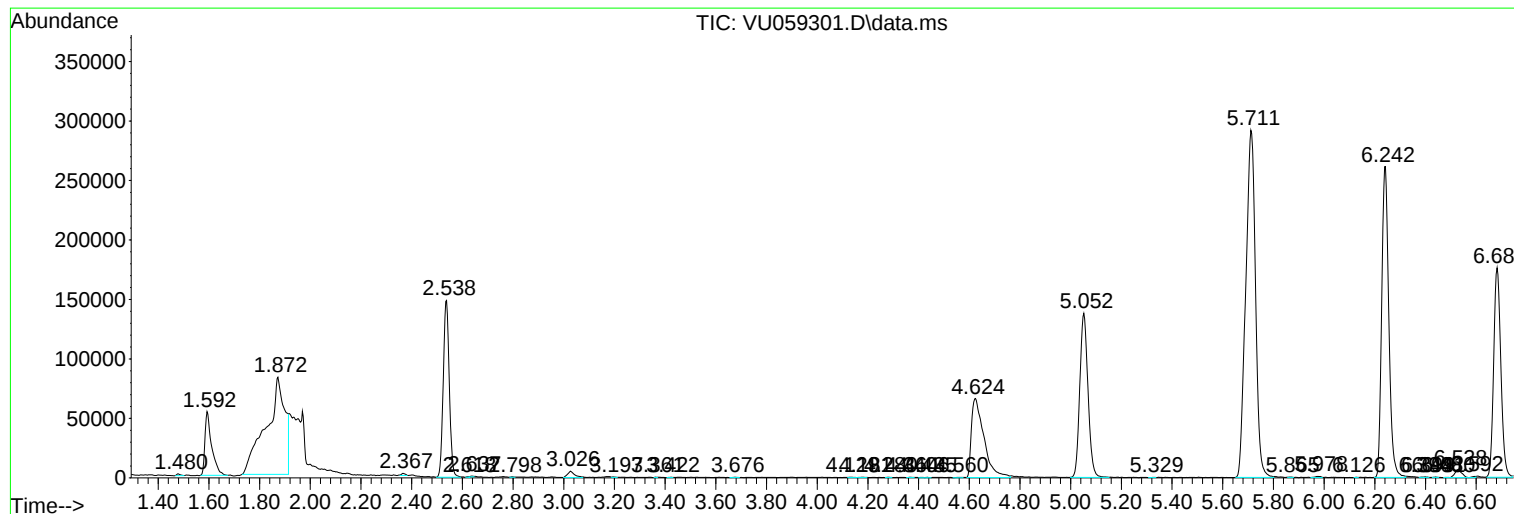
Sum of corrected areas: 6524389

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059301.D
Acq On : 18 Jun 2024 10:57
Operator : MD/SY
Sample : P2850-08ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB09ME

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\VU061824\
Data File : VU059301.D
Acq On : 18 Jun 2024 10:57
Operator : MD/SY
Sample : P2850-08ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB09ME

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\VU061824\
Data File : VU059301.D
Acq On : 18 Jun 2024 10:57
Operator : MD/SY
Sample : P2850-08ME
Misc : 4.94g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB09ME

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	--Internal Standard--
				#	RT Resp Conc