

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
 Data File : VU059055.D
 Acq On : 29 May 2024 16:50
 Operator : MD/SY
 Sample : P2588-07ME
 Misc : 5.87g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5S6ME

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: VU059055.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	53	59	65	rBV	5822	6345	0.94%	0.115%
2	1.592	87	94	116	rVB	45407	74695	11.05%	1.354%
3	1.875	138	182	198	rBV4	98962	625747	92.60%	11.339%
4	2.534	376	387	402	rBV	105143	170451	25.22%	3.089%
5	2.936	510	512	514	rBV3	624	298	0.04%	0.005%
6	3.023	530	539	550	rBV4	5252	11079	1.64%	0.201%
7	3.107	563	565	569	rVB3	457	265	0.04%	0.005%
8	3.171	570	585	596	rBV	6943	15713	2.33%	0.285%
9	3.261	610	613	617	rVB4	406	271	0.04%	0.005%
10	3.631	725	728	735	rVB2	381	510	0.08%	0.009%
11	3.673	735	741	742	rBV2	689	621	0.09%	0.011%
12	3.776	768	773	776	rBV	263	250	0.04%	0.005%
13	4.460	981	986	990	rBV2	150	177	0.03%	0.003%
14	4.499	994	998	1000	rBV	322	249	0.04%	0.005%
15	4.573	1018	1021	1026	rBV	192	209	0.03%	0.004%
16	4.624	1026	1037	1077	rBV2	47079	156720	23.19%	2.840%
17	4.875	1113	1115	1122	rVB3	395	405	0.06%	0.007%
18	4.962	1139	1142	1146	rVB2	243	188	0.03%	0.003%
19	5.049	1152	1169	1197	rBV	96011	222488	32.92%	4.032%
20	5.158	1200	1203	1206	rBV3	300	184	0.03%	0.003%
21	5.274	1233	1239	1245	rVB2	306	414	0.06%	0.008%
22	5.309	1245	1250	1253	rBV2	252	266	0.04%	0.005%
23	5.361	1261	1266	1268	rBV2	259	223	0.03%	0.004%
24	5.460	1294	1297	1304	rBV	280	372	0.06%	0.007%
25	5.711	1350	1375	1400	rBV2	207506	550070	81.40%	9.968%
26	5.981	1448	1459	1471	rBV6	2055	4955	0.73%	0.090%
27	6.155	1510	1513	1516	rBV2	207	224	0.03%	0.004%
28	6.238	1527	1539	1562	rBV	277240	545481	80.72%	9.885%
29	6.399	1584	1589	1593	rVB3	261	263	0.04%	0.005%
30	6.435	1595	1600	1607	rVB3	273	345	0.05%	0.006%
31	6.528	1619	1629	1641	rVB3	3843	8669	1.28%	0.157%
32	6.595	1641	1650	1664	rBV4	3012	7133	1.06%	0.129%
33	6.682	1664	1677	1700	rBV	128096	255581	37.82%	4.631%
34	6.814	1715	1718	1723	rVB2	225	190	0.03%	0.003%
35	6.888	1737	1741	1746	rVB	250	248	0.04%	0.004%
36	7.055	1789	1793	1797	rVB	255	210	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
 Data File : VU059055.D
 Acq On : 29 May 2024 16:50
 Operator : MD/SY
 Sample : P2588-07ME
 Misc : 5.87g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5S6ME

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	7.213	1832	1842	1843	rBV3	1150	1173	0.17%	0.021%
38	7.422	1904	1907	1913	rVV2	201	214	0.03%	0.004%
39	7.483	1922	1926	1928	rBV2	303	253	0.04%	0.005%
40	7.499	1928	1931	1936	rVV3	314	348	0.05%	0.006%
41	7.560	1939	1950	1971	rVB	63665	118788	17.58%	2.153%
42	7.682	1984	1988	1992	rVB2	356	334	0.05%	0.006%
43	7.708	1992	1996	1999	rBV	253	218	0.03%	0.004%
44	7.785	2014	2020	2027	rVB3	667	935	0.14%	0.017%
45	7.817	2027	2030	2033	rBV	285	259	0.04%	0.005%
46	7.891	2040	2053	2075	rBV	225224	398540	58.98%	7.222%
47	7.984	2076	2082	2087	rVV7	1456	2117	0.31%	0.038%
48	8.132	2125	2128	2131	rBV2	288	238	0.04%	0.004%
49	8.177	2131	2142	2171	rVV2	41748	80182	11.87%	1.453%
50	8.415	2214	2216	2223	rVB2	295	326	0.05%	0.006%
51	8.463	2227	2231	2232	rBV	226	185	0.03%	0.003%
52	8.553	2254	2259	2261	rBV2	567	442	0.07%	0.008%
53	8.582	2265	2268	2273	rBV	290	274	0.04%	0.005%
54	8.647	2273	2288	2325	rBV	116928	320618	47.45%	5.810%
55	8.862	2353	2355	2358	rVV	449	298	0.04%	0.005%
56	8.885	2360	2362	2366	rVB2	331	187	0.03%	0.003%
57	8.920	2370	2373	2377	rVB3	488	330	0.05%	0.006%
58	8.943	2377	2380	2385	rBV3	222	177	0.03%	0.003%
59	9.042	2404	2411	2413	rBV	337	396	0.06%	0.007%
60	9.415	2513	2527	2549	rBV	372580	675745	100.00%	12.245%
61	9.573	2572	2576	2584	rVB4	1112	1524	0.23%	0.028%
62	9.698	2607	2615	2627	rBV4	2426	3919	0.58%	0.071%
63	9.811	2645	2650	2656	rVB2	177	249	0.04%	0.005%
64	9.885	2669	2673	2676	rBV2	252	219	0.03%	0.004%
65	9.965	2695	2698	2701	rBV2	356	344	0.05%	0.006%
66	10.113	2736	2744	2750	rBV3	852	1235	0.18%	0.022%
67	10.142	2750	2753	2755	rVV	332	180	0.03%	0.003%
68	10.377	2823	2826	2829	rBV	277	249	0.04%	0.005%
69	10.454	2846	2850	2855	rVV	363	238	0.04%	0.004%
70	10.486	2855	2860	2863	rBV2	367	363	0.05%	0.007%
71	10.553	2876	2881	2884	rBV2	299	351	0.05%	0.006%
72	10.756	2931	2944	2969	rVB	191641	328786	48.66%	5.958%
73	10.856	2969	2975	2978	rBV3	422	489	0.07%	0.009%
74	10.933	2993	2999	3004	rBV2	232	220	0.03%	0.004%
75	11.100	3045	3051	3055	rBV3	413	571	0.08%	0.010%
76	11.190	3076	3079	3083	rBV	223	184	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
 Data File : VU059055.D
 Acq On : 29 May 2024 16:50
 Operator : MD/SY
 Sample : P2588-07ME
 Misc : 5.87g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5S6ME

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	11.331	3121	3123	3129	rVB2	336	183	0.03%	0.003%
78	11.389	3133	3141	3144	rBV2	362	427	0.06%	0.008%
79	11.463	3160	3164	3166	rBV2	219	183	0.03%	0.003%
80	11.643	3217	3220	3223	rBV	244	215	0.03%	0.004%
81	11.714	3238	3242	3247	rBV2	314	408	0.06%	0.007%
82	11.749	3251	3253	3256	rVV2	505	300	0.04%	0.005%
83	11.811	3261	3272	3301	rVV	348595	566372	83.81%	10.263%
84	11.965	3318	3320	3323	rBV2	529	302	0.04%	0.005%
85	12.042	3341	3344	3346	rBV	266	184	0.03%	0.003%
86	12.190	3378	3390	3414	rBV	198762	337832	49.99%	6.122%
87	12.341	3435	3437	3442	rVB2	256	200	0.03%	0.004%
88	12.553	3500	3503	3505	rBV	327	196	0.03%	0.004%
89	13.290	3729	3732	3734	rBV2	286	213	0.03%	0.004%
90	13.415	3768	3771	3772	rBV	357	195	0.03%	0.004%
91	13.897	3918	3921	3927	rBV2	526	475	0.07%	0.009%
92	13.929	3927	3931	3933	rBV	398	333	0.05%	0.006%
93	14.113	3977	3988	4003	rBV3	1425	3642	0.54%	0.066%
94	14.299	4043	4046	4049	rBV2	429	283	0.04%	0.005%
95	14.341	4052	4059	4065	rVB3	501	919	0.14%	0.017%
96	14.486	4099	4104	4107	rBV	676	509	0.08%	0.009%
97	14.672	4153	4162	4169	rBV2	465	974	0.14%	0.018%
98	14.884	4223	4228	4229	rBV2	423	321	0.05%	0.006%
99	14.952	4246	4249	4253	rBV2	307	302	0.04%	0.005%
100	16.129	4612	4615	4616	rBV2	460	292	0.04%	0.005%

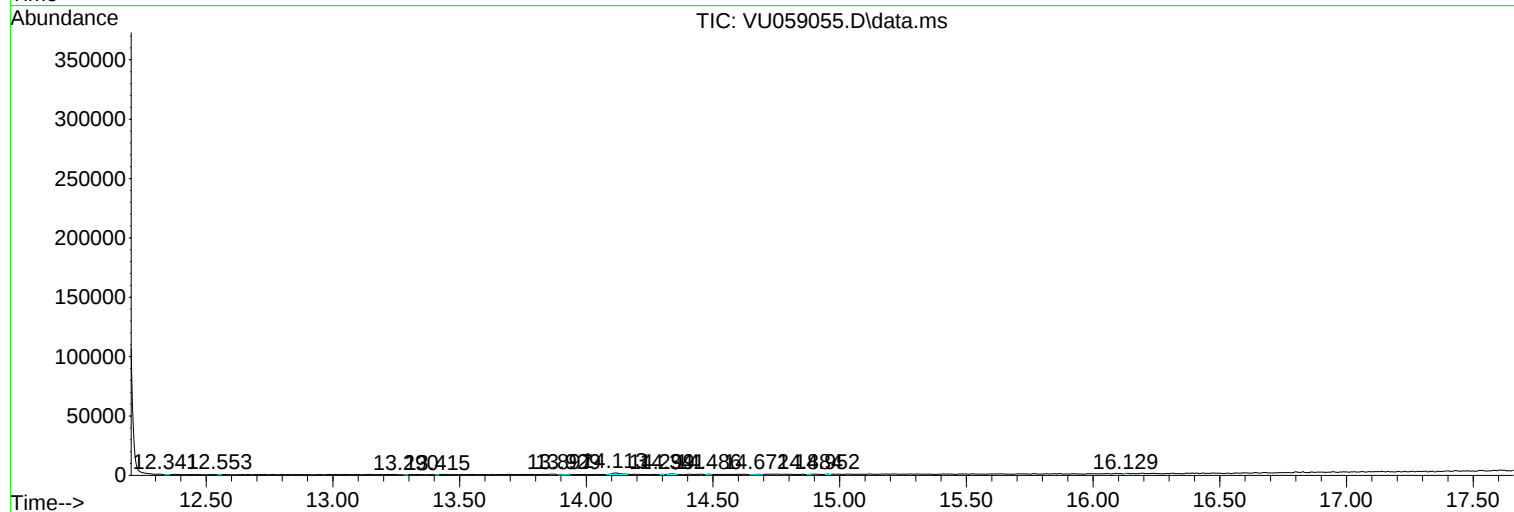
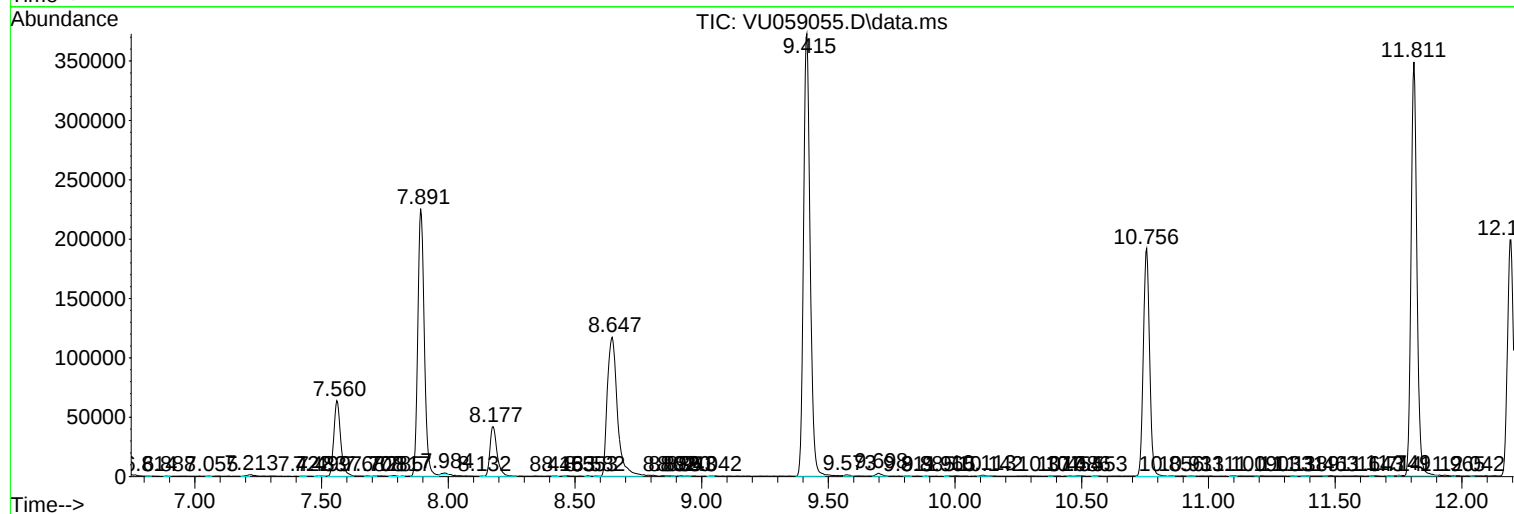
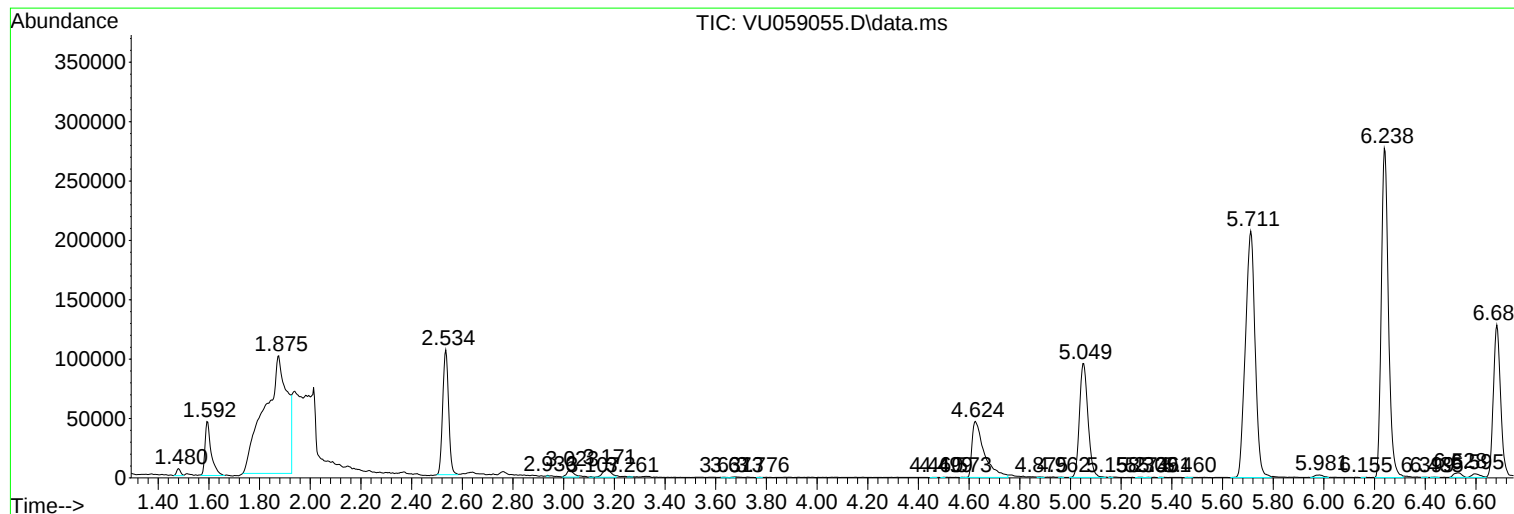
Sum of corrected areas: 5518467

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052924\
Data File : VU059055.D
Acq On : 29 May 2024 16:50
Operator : MD/SY
Sample : P2588-07ME
Misc : 5.87g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5S6ME

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 : VU059055.D
Acq On : 29 May 2024 16:50
Operator : MD/SY
Sample : P2588-07ME
Misc : 5.87g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5S6ME

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 : VU059055.D
Acq On : 29 May 2024 16:50
Operator : MD/SY
Sample : P2588-07ME
Misc : 5.87g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5S6ME

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