

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052824\
 Data File : VU059029.D
 Acq On : 28 May 2024 14:51
 Operator : MD/SY
 Sample : P2571-13ME
 Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH667ME

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\SFAMULM052324WMA.M
 Title : VOC Analysis

Signal : TIC: VU059029.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	rBV2	5137	5320	0.64%	0.086%
2	1.592	86	94	119	rVB	73633	120077	14.55%	1.935%
3	1.830	137	168	169	rBV3	61131	228789	27.73%	3.687%
4	2.534	374	387	403	rBV	158780	262629	31.83%	4.232%
5	3.026	532	540	552	rVB3	4441	8098	0.98%	0.130%
6	3.084	556	558	564	rVB3	868	695	0.08%	0.011%
7	3.110	564	566	568	rBV	405	216	0.03%	0.003%
8	3.168	570	584	600	rBV	4432	12149	1.47%	0.196%
9	3.242	605	607	615	rVB3	732	665	0.08%	0.011%
10	3.287	618	621	624	rBV2	506	277	0.03%	0.004%
11	3.351	636	641	646	rBV2	523	452	0.05%	0.007%
12	3.628	724	727	731	rVB	313	214	0.03%	0.003%
13	3.669	734	740	742	rBV3	741	670	0.08%	0.011%
14	3.901	807	812	817	rBV	259	291	0.04%	0.005%
15	4.017	842	848	852	rBV2	216	261	0.03%	0.004%
16	4.046	852	857	859	rBV	253	254	0.03%	0.004%
17	4.161	887	893	898	rBV2	329	308	0.04%	0.005%
18	4.251	914	921	925	rBV2	203	255	0.03%	0.004%
19	4.422	970	974	977	rBV	216	218	0.03%	0.004%
20	4.621	1025	1036	1078	rBV	65133	207706	25.17%	3.347%
21	4.862	1108	1111	1114	rBV2	317	195	0.02%	0.003%
22	5.049	1154	1169	1196	rBV	136600	315756	38.27%	5.088%
23	5.287	1240	1243	1248	rVB2	226	196	0.02%	0.003%
24	5.316	1249	1252	1256	rVB2	279	196	0.02%	0.003%
25	5.383	1269	1273	1276	rBV	222	224	0.03%	0.004%
26	5.599	1336	1340	1344	rBV2	317	312	0.04%	0.005%
27	5.711	1356	1375	1410	rBV3	311742	825117	100.00%	13.295%
28	5.920	1434	1440	1443	rVB2	326	324	0.04%	0.005%
29	5.968	1448	1455	1457	rBV4	2329	2332	0.28%	0.038%
30	6.174	1513	1519	1523	rVB2	273	264	0.03%	0.004%
31	6.238	1526	1539	1567	rBV	252895	498243	60.38%	8.028%
32	6.525	1619	1628	1637	rBV7	3768	6923	0.84%	0.112%
33	6.605	1641	1653	1663	rBV4	2735	6146	0.74%	0.099%
34	6.679	1664	1676	1700	rVB2	184639	373047	45.21%	6.011%
35	6.811	1713	1717	1719	rBV	581	458	0.06%	0.007%
36	6.827	1719	1722	1725	rVV2	600	411	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052824\
 Data File : VU059029.D
 Acq On : 28 May 2024 14:51
 Operator : MD/SY
 Sample : P2571-13ME
 Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH667ME

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\SFAMULM052324WMA.M
 Title : VOC Analysis

37	7.190	1831	1835	1838	rBV2	284	244	0.03%	0.004%
38	7.216	1838	1843	1850	rVB6	998	1377	0.17%	0.022%
39	7.267	1856	1859	1868	rBV2	169	226	0.03%	0.004%
40	7.325	1874	1877	1881	rBV2	313	247	0.03%	0.004%
41	7.447	1911	1915	1922	rBV	204	208	0.03%	0.003%
42	7.486	1922	1927	1929	rBV2	444	367	0.04%	0.006%
43	7.502	1929	1932	1936	rVB2	382	241	0.03%	0.004%
44	7.560	1936	1950	1974	rBV	91540	171011	20.73%	2.756%
45	7.650	1974	1978	1982	rVB3	243	196	0.02%	0.003%
46	7.891	2039	2053	2075	rBV	335356	594186	72.01%	9.574%
47	7.991	2078	2084	2085	rBV3	1509	1622	0.20%	0.026%
48	8.087	2111	2114	2118	rVB2	311	237	0.03%	0.004%
49	8.116	2118	2123	2127	rVB2	249	280	0.03%	0.005%
50	8.174	2130	2141	2160	rBV	60593	115037	13.94%	1.854%
51	8.351	2191	2196	2199	rVV3	396	363	0.04%	0.006%
52	8.467	2227	2232	2241	rVB2	428	542	0.07%	0.009%
53	8.544	2248	2256	2260	rBV2	240	246	0.03%	0.004%
54	8.643	2273	2287	2317	rBV	162118	430718	52.20%	6.940%
55	8.814	2336	2340	2344	rVB4	614	541	0.07%	0.009%
56	8.920	2369	2373	2375	rVB	522	310	0.04%	0.005%
57	8.988	2390	2394	2402	rVB2	392	390	0.05%	0.006%
58	9.020	2402	2404	2407	rVB	362	189	0.02%	0.003%
59	9.042	2407	2411	2414	rBV2	449	355	0.04%	0.006%
60	9.261	2476	2479	2485	rVB	289	273	0.03%	0.004%
61	9.293	2485	2489	2492	rBV2	325	248	0.03%	0.004%
62	9.412	2514	2526	2563	rVV	335127	613533	74.36%	9.886%
63	9.541	2563	2566	2571	rVB2	235	226	0.03%	0.004%
64	9.705	2607	2617	2626	rBV3	1621	3050	0.37%	0.049%
65	10.113	2738	2744	2746	rBV	402	411	0.05%	0.007%
66	10.242	2780	2784	2789	rBV2	265	241	0.03%	0.004%
67	10.396	2827	2832	2838	rVB2	250	272	0.03%	0.004%
68	10.756	2931	2944	2968	rVV	249058	424445	51.44%	6.839%
69	10.888	2982	2985	2992	rVB2	452	525	0.06%	0.008%
70	11.058	3035	3038	3043	rVB	285	226	0.03%	0.004%
71	11.084	3043	3046	3053	rBV2	225	276	0.03%	0.004%
72	11.113	3053	3055	3063	rBV3	581	565	0.07%	0.009%
73	11.216	3083	3087	3093	rBV2	360	490	0.06%	0.008%
74	11.450	3156	3160	3167	rBV2	210	298	0.04%	0.005%
75	11.605	3204	3208	3213	rBV2	323	251	0.03%	0.004%
76	11.708	3237	3240	3243	rVV2	264	191	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052824\
 Data File : VU059029.D
 Acq On : 28 May 2024 14:51
 Operator : MD/SY
 Sample : P2571-13ME
 Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH667ME

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\SFAMULM052324WMA.M
 Title : VOC Analysis

77	11.753	3251	3254	3260	rBV2	252	244	0.03%	0.004%
78	11.811	3260	3272	3292	rBV	298920	487021	59.02%	7.848%
79	11.920	3303	3306	3308	rVB3	486	267	0.03%	0.004%
80	12.071	3351	3353	3358	rVB	365	240	0.03%	0.004%
81	12.190	3378	3390	3413	rBV	281258	469040	56.85%	7.558%
82	12.328	3431	3433	3436	rVB3	432	219	0.03%	0.004%
83	12.364	3442	3444	3447	rVB	377	199	0.02%	0.003%
84	12.746	3560	3563	3566	rBV2	345	249	0.03%	0.004%
85	12.920	3614	3617	3622	rVB2	296	231	0.03%	0.004%
86	12.955	3625	3628	3631	rBV2	288	243	0.03%	0.004%
87	13.466	3784	3787	3792	rVB	496	360	0.04%	0.006%
88	13.492	3792	3795	3798	rBV	240	192	0.02%	0.003%
89	13.531	3804	3807	3811	rVB	318	196	0.02%	0.003%
90	13.573	3817	3820	3823	rBV	370	309	0.04%	0.005%
91	13.737	3868	3871	3874	rVB2	338	213	0.03%	0.003%
92	13.952	3935	3938	3941	rBV2	351	225	0.03%	0.004%
93	14.254	4029	4032	4036	rBV	293	227	0.03%	0.004%
94	14.415	4079	4082	4086	rBV2	322	261	0.03%	0.004%
95	14.437	4086	4089	4091	rBV	312	215	0.03%	0.003%
96	14.769	4189	4192	4194	rBV3	425	310	0.04%	0.005%
97	15.026	4270	4272	4278	rVB	489	327	0.04%	0.005%
98	15.109	4295	4298	4301	rBV2	408	321	0.04%	0.005%
99	15.547	4431	4434	4436	rBV2	464	299	0.04%	0.005%
100	16.161	4623	4625	4627	rBV2	488	286	0.03%	0.005%

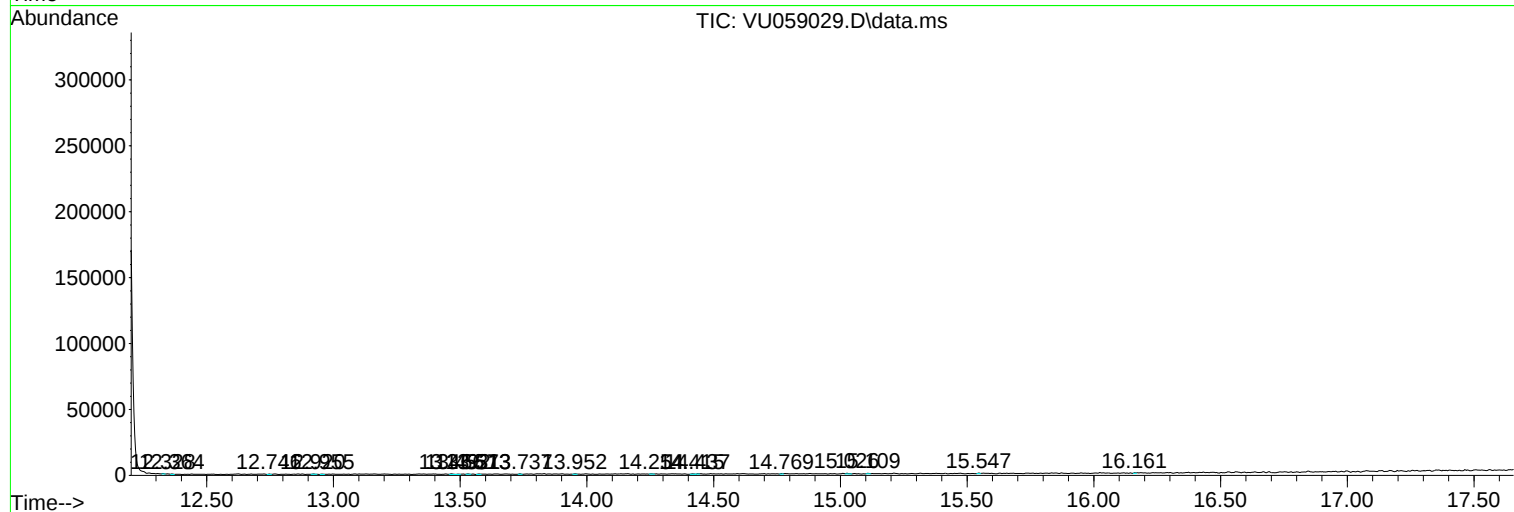
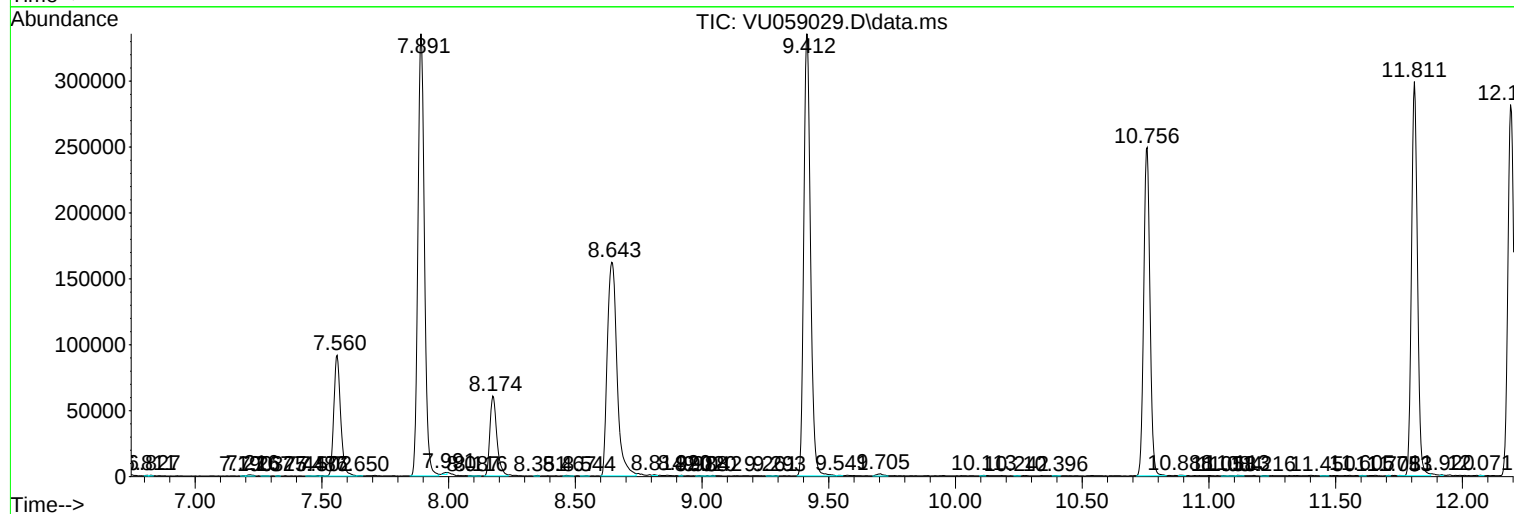
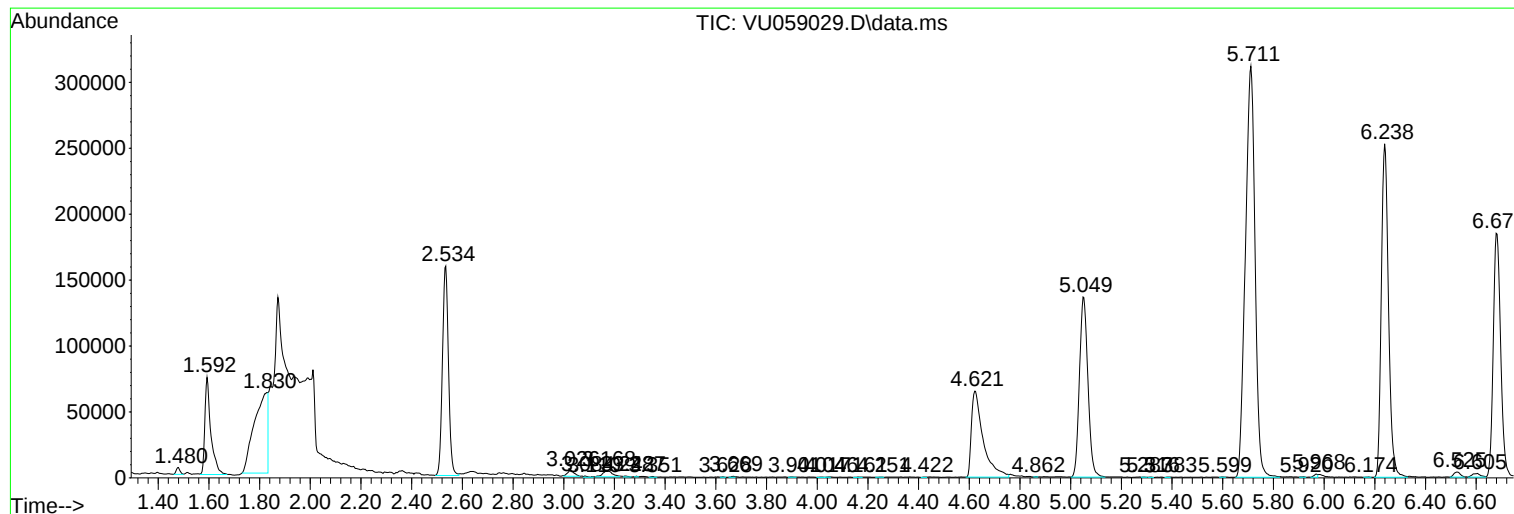
Sum of corrected areas: 6206036

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052824\
Data File : VU059029.D
Acq On : 28 May 2024 14:51
Operator : MD/SY
Sample : P2571-13ME
Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH667ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052824\
Data File : VU059029.D
Acq On : 28 May 2024 14:51
Operator : MD/SY
Sample : P2571-13ME
Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH667ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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\VU052824\
Data File : VU059029.D
Acq On : 28 May 2024 14:51
Operator : MD/SY
Sample : P2571-13ME
Misc : 4.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH667ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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
------------------	----	---------	-------	----------	---	----	------	------