

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
 Data File : VU059958.D
 Acq On : 15 Jul 2024 17:54
 Operator : MD/SY
 Sample : P3230-03ME 200X
 Misc : 5.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB34ME

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\SFAMULM070224WMA.M
 Title : VOC Analysis

Signal : TIC: VU059958.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	88	95	114	rVB	61464	77150	12.40%	1.392%
2	1.901	183	190	207	rVB	46358	67344	10.82%	1.215%
3	2.557	383	394	412	rBV	101088	165674	26.62%	2.989%
4	2.769	456	460	462	rBV2	328	273	0.04%	0.005%
5	3.039	535	544	554	rVB4	1891	3384	0.54%	0.061%
6	3.181	574	588	603	rBV	4832	10714	1.72%	0.193%
7	3.547	699	702	705	rBV2	162	130	0.02%	0.002%
8	3.654	729	735	738	rBV2	197	233	0.04%	0.004%
9	3.699	746	749	751	rVB	244	134	0.02%	0.002%
10	3.711	751	753	755	rBV2	150	84	0.01%	0.002%
11	3.991	837	840	846	rVB2	220	225	0.04%	0.004%
12	4.030	849	852	856	rVB2	160	114	0.02%	0.002%
13	4.056	856	860	861	rBV2	196	119	0.02%	0.002%
14	4.168	892	895	897	rBV	133	73	0.01%	0.001%
15	4.309	937	939	941	rBV	91	54	0.01%	0.001%
16	4.374	954	959	962	rBV	214	238	0.04%	0.004%
17	4.512	992	1002	1005	rBV2	224	339	0.05%	0.006%
18	4.547	1010	1013	1015	rBV2	188	118	0.02%	0.002%
19	4.564	1015	1018	1023	rBV2	180	142	0.02%	0.003%
20	4.618	1025	1035	1070	rBV	70343	188276	30.25%	3.397%
21	4.991	1148	1151	1154	rBV2	207	124	0.02%	0.002%
22	5.055	1156	1171	1196	rVV	107841	238419	38.31%	4.302%
23	5.252	1230	1232	1235	rVB	223	120	0.02%	0.002%
24	5.271	1235	1238	1240	rVB2	131	64	0.01%	0.001%
25	5.290	1240	1244	1247	rBV2	508	381	0.06%	0.007%
26	5.306	1247	1249	1255	rVB2	232	203	0.03%	0.004%
27	5.371	1266	1269	1270	rBV	78	45	0.01%	0.001%
28	5.428	1281	1287	1289	rBV	199	206	0.03%	0.004%
29	5.506	1307	1311	1316	rBV2	165	214	0.03%	0.004%
30	5.541	1316	1322	1324	rVB2	271	288	0.05%	0.005%
31	5.557	1324	1327	1332	rBV2	189	174	0.03%	0.003%
32	5.637	1349	1352	1357	rBV2	165	137	0.02%	0.002%
33	5.721	1357	1378	1400	rBV2	206086	568482	91.34%	10.257%
34	5.998	1462	1464	1468	rBV	135	109	0.02%	0.002%
35	6.030	1472	1474	1475	rBV	183	82	0.01%	0.001%
36	6.088	1490	1492	1494	rBV	64	36	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
 Data File : VU059958.D
 Acq On : 15 Jul 2024 17:54
 Operator : MD/SY
 Sample : P3230-03ME 200X
 Misc : 5.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB34ME

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\SFAMULM070224WMA.M
 Title : VOC Analysis

37	6.133	1503	1506	1508	rBV	186	127	0.02%	0.002%
38	6.245	1528	1541	1563	rBV	251592	482976	77.61%	8.715%
39	6.451	1603	1605	1609	rBV	270	202	0.03%	0.004%
40	6.538	1623	1632	1648	rVB6	7676	15696	2.52%	0.283%
41	6.608	1648	1654	1660	rVB2	221	326	0.05%	0.006%
42	6.686	1660	1678	1703	rBV	134218	266538	42.83%	4.809%
43	6.805	1713	1715	1718	rBV2	195	96	0.02%	0.002%
44	6.834	1720	1724	1727	rBV2	204	174	0.03%	0.003%
45	7.017	1779	1781	1786	rVB2	171	89	0.01%	0.002%
46	7.284	1860	1864	1867	rBV	185	146	0.02%	0.003%
47	7.322	1873	1876	1878	rVB2	119	63	0.01%	0.001%
48	7.342	1878	1882	1886	rVB2	297	253	0.04%	0.005%
49	7.361	1886	1888	1890	rBV2	61	36	0.01%	0.001%
50	7.473	1916	1923	1926	rBV2	266	325	0.05%	0.006%
51	7.499	1926	1931	1933	rBV	127	122	0.02%	0.002%
52	7.518	1934	1937	1940	rBV2	181	143	0.02%	0.003%
53	7.563	1940	1951	1967	rBV	65527	116466	18.71%	2.101%
54	7.679	1985	1987	1992	rVB3	400	298	0.05%	0.005%
55	7.708	1992	1996	1999	rBV	368	344	0.06%	0.006%
56	7.779	2013	2018	2021	rBV2	168	151	0.02%	0.003%
57	7.895	2035	2054	2075	rBV	229397	401364	64.49%	7.242%
58	8.129	2123	2127	2129	rBV	158	144	0.02%	0.003%
59	8.178	2132	2142	2161	rVV2	45830	79331	12.75%	1.431%
60	8.280	2173	2174	2176	rBV2	110	26	0.00%	0.000%
61	8.313	2182	2184	2188	rVB2	182	71	0.01%	0.001%
62	8.370	2200	2202	2205	rVB2	189	71	0.01%	0.001%
63	8.550	2239	2258	2273	rBV	371334	622085	99.96%	11.224%
64	8.631	2273	2283	2313	rVB	182831	337775	54.27%	6.095%
65	9.104	2425	2430	2433	rBV2	287	253	0.04%	0.005%
66	9.313	2493	2495	2498	rBV	97	60	0.01%	0.001%
67	9.415	2515	2527	2552	rBV	365853	622347	100.00%	11.229%
68	9.689	2609	2612	2613	rBV	498	255	0.04%	0.005%
69	9.756	2630	2633	2634	rBV	85	45	0.01%	0.001%
70	10.149	2752	2755	2760	rBV2	287	249	0.04%	0.004%
71	10.213	2771	2775	2777	rBV	158	127	0.02%	0.002%
72	10.753	2930	2943	2963	rBV	223210	368302	59.18%	6.645%
73	10.930	2995	2998	3000	rBV	153	97	0.02%	0.002%
74	10.981	3011	3014	3017	rBV	187	141	0.02%	0.003%
75	11.026	3025	3028	3029	rBV	169	102	0.02%	0.002%
76	11.811	3260	3272	3292	rBV	316322	518945	83.39%	9.364%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
Data File : VU059958.D
Acq On : 15 Jul 2024 17:54
Operator : MD/SY
Sample : P3230-03ME 200X
Misc : 5.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB34ME

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\SFAMULM070224WMA.M

Title : VOC Analysis

77	12.026	3335	3339	3340	rBV	329	230	0.04%	0.004%
78	12.190	3378	3390	3409	rBV	225422	381382	61.28%	6.881%
79	12.380	3446	3449	3454	rVB	458	333	0.05%	0.006%

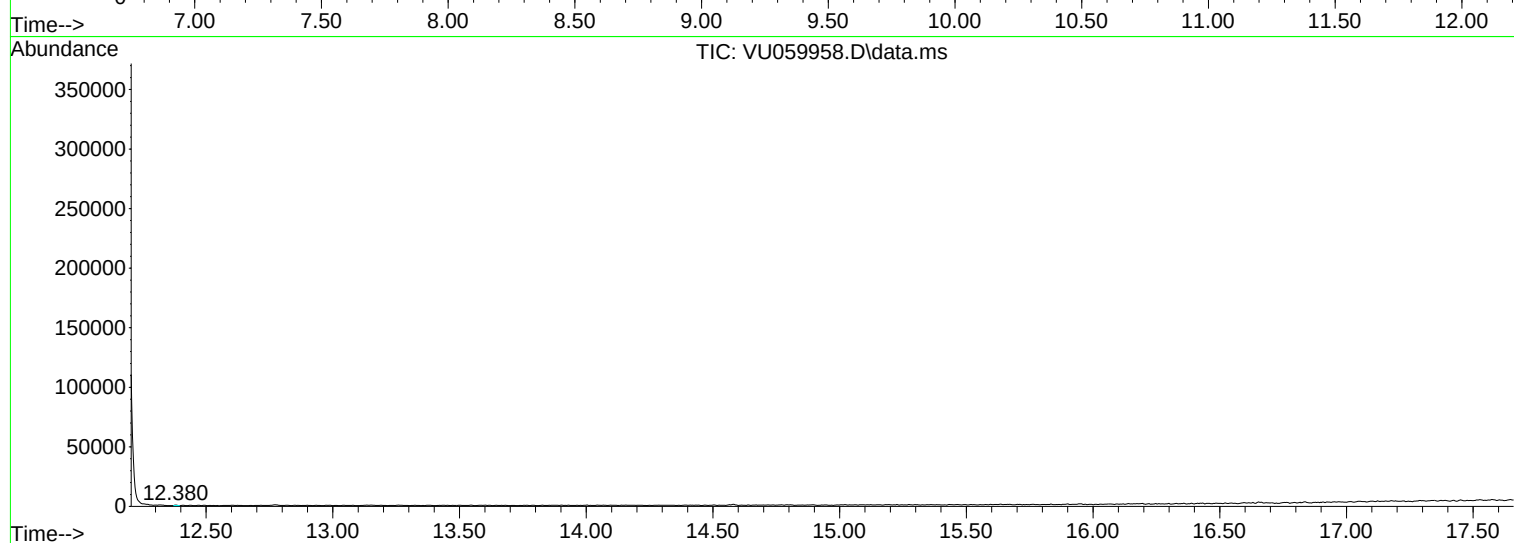
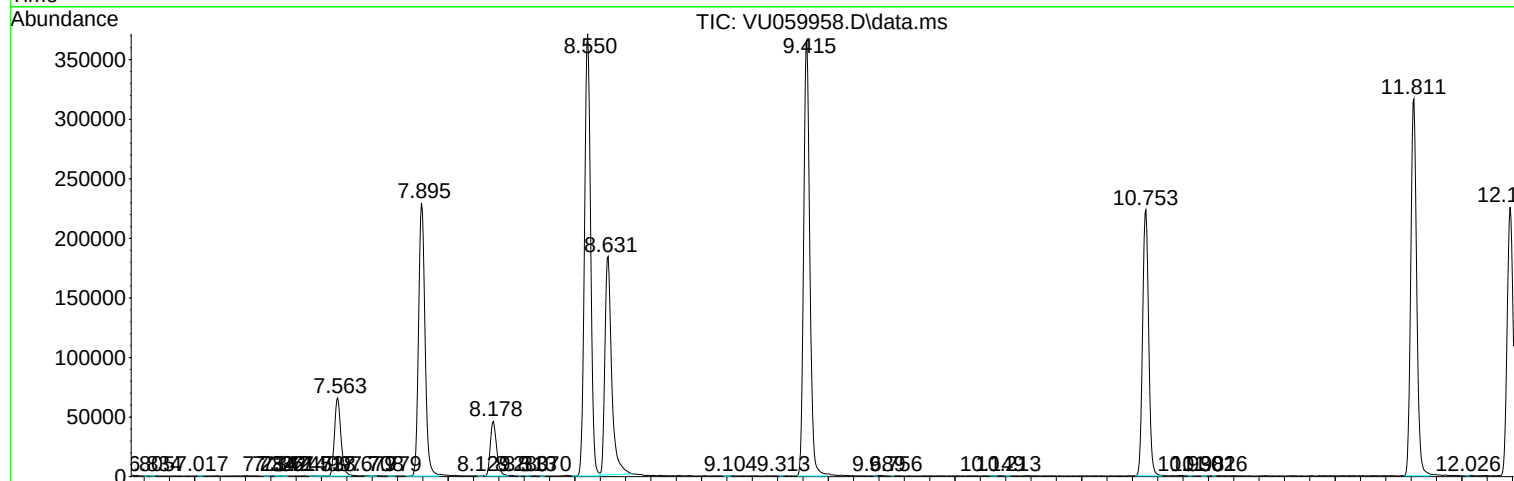
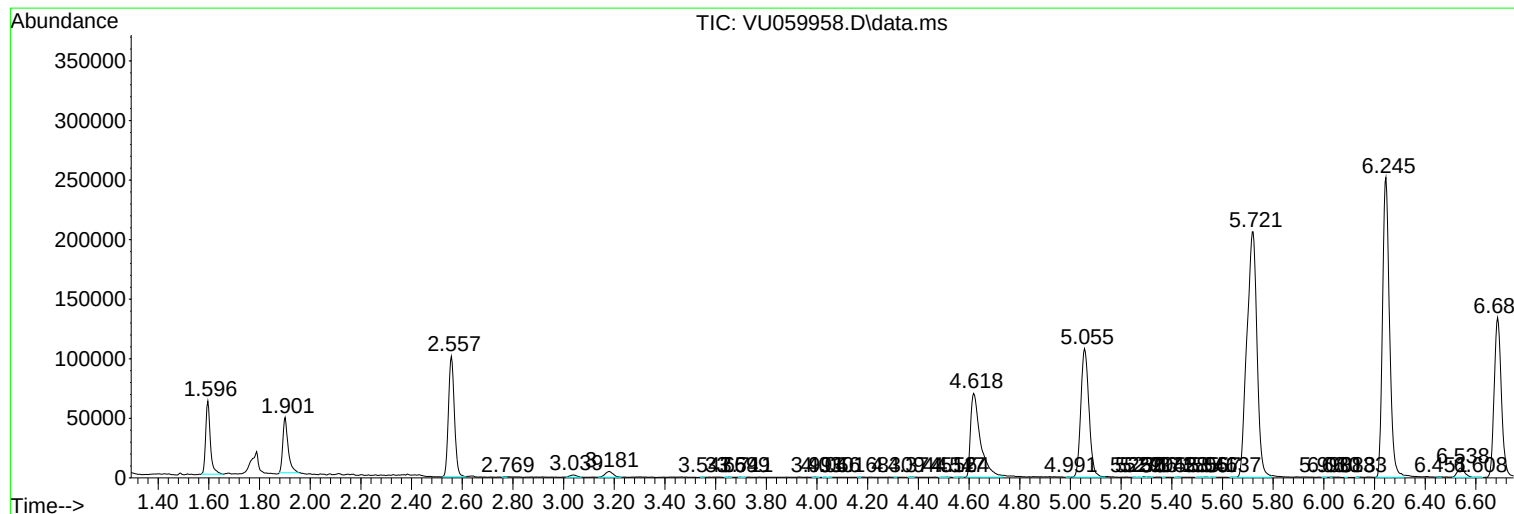
Sum of corrected areas: 5542208

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
Data File : VU059958.D
Acq On : 15 Jul 2024 17:54
Operator : MD/SY
Sample : P3230-03ME 200X
Misc : 5.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB34ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071524\
Data File : VU059958.D
Acq On : 15 Jul 2024 17:54
Operator : MD/SY
Sample : P3230-03ME 200X
Misc : 5.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB34ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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\VU071524\
Data File : VU059958.D
Acq On : 15 Jul 2024 17:54
Operator : MD/SY
Sample : P3230-03ME 200X
Misc : 5.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB34ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM070224WMA.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