

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053514.D
 Acq On : 03 Apr 2023 12:54
 Operator : JC/MD
 Sample : 02121-07ME 5X
 Misc : 5.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1180ME

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\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053514.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	95	rVB	101104	114135	13.05%	1.682%
2	1.896	167	173	187	rVB	77906	105855	12.10%	1.560%
3	2.559	368	379	393	rBV	149461	248211	28.38%	3.657%
4	3.041	522	529	537	rVB5	1888	3311	0.38%	0.049%
5	3.176	566	571	576	rBV2	754	924	0.11%	0.014%
6	3.346	614	624	636	rBV3	5416	9802	1.12%	0.144%
7	3.658	717	721	727	rBV2	254	318	0.04%	0.005%
8	3.706	733	736	737	rBV2	230	118	0.01%	0.002%
9	3.864	782	785	786	rBV2	162	83	0.01%	0.001%
10	4.433	959	962	964	rBV	279	132	0.02%	0.002%
11	4.449	964	967	970	rVB2	234	149	0.02%	0.002%
12	4.616	1006	1019	1021	rBV	67416	107684	12.31%	1.587%
13	4.890	1102	1104	1109	rVB	207	115	0.01%	0.002%
14	5.054	1140	1155	1177	rBV2	142845	319221	36.49%	4.703%
15	5.173	1187	1192	1195	rBV3	453	527	0.06%	0.008%
16	5.337	1242	1243	1248	rBV2	191	124	0.01%	0.002%
17	5.382	1253	1257	1259	rBV2	193	169	0.02%	0.002%
18	5.439	1273	1275	1278	rVB2	200	125	0.01%	0.002%
19	5.719	1341	1362	1384	rBV2	278671	756141	86.45%	11.141%
20	5.883	1411	1413	1417	rVB	383	170	0.02%	0.003%
21	5.944	1430	1432	1435	rBV	151	110	0.01%	0.002%
22	5.970	1439	1440	1442	rBV	343	158	0.02%	0.002%
23	6.044	1458	1463	1465	rVB2	387	247	0.03%	0.004%
24	6.243	1509	1525	1543	rBV	323213	612885	70.07%	9.030%
25	6.488	1598	1601	1603	rBV2	184	104	0.01%	0.002%
26	6.526	1603	1613	1625	rVV7	4315	9127	1.04%	0.134%
27	6.684	1649	1662	1687	rBV	178040	344295	39.36%	5.073%
28	6.873	1719	1721	1725	rBV2	175	130	0.01%	0.002%
29	6.954	1744	1746	1750	rVV	194	115	0.01%	0.002%
30	6.992	1756	1758	1761	rBV	219	161	0.02%	0.002%
31	7.086	1783	1787	1788	rBV	208	176	0.02%	0.003%
32	7.185	1812	1818	1823	rBV4	910	1183	0.14%	0.017%
33	7.311	1854	1857	1858	rBV	187	128	0.01%	0.002%
34	7.465	1901	1905	1906	rBV	153	104	0.01%	0.002%
35	7.494	1910	1914	1916	rBV2	285	191	0.02%	0.003%
36	7.558	1922	1934	1954	rBV	103247	180779	20.67%	2.664%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053514.D
 Acq On : 03 Apr 2023 12:54
 Operator : JC/MD
 Sample : 02121-07ME 5X
 Misc : 5.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1180ME

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\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.690	1970	1975	1979	rBV5	744	842	0.10%	0.012%
38	7.806	2007	2011	2013	rBV	260	178	0.02%	0.003%
39	7.893	2025	2038	2058	rBV	363019	629415	71.96%	9.274%
40	8.047	2083	2086	2088	rBV2	293	155	0.02%	0.002%
41	8.063	2088	2091	2095	rBV2	282	236	0.03%	0.003%
42	8.176	2115	2126	2146	rVB	74297	122685	14.03%	1.808%
43	8.288	2159	2161	2164	rVB2	274	154	0.02%	0.002%
44	8.314	2164	2169	2175	rVB2	458	595	0.07%	0.009%
45	8.353	2178	2181	2185	rBV	137	126	0.01%	0.002%
46	8.517	2231	2232	2234	rBV	293	140	0.02%	0.002%
47	8.629	2255	2267	2294	rBV	193291	354623	40.54%	5.225%
48	8.787	2314	2316	2317	rBV	347	162	0.02%	0.002%
49	8.825	2325	2328	2330	rBV2	249	169	0.02%	0.002%
50	8.886	2344	2347	2349	rBV	239	132	0.02%	0.002%
51	8.925	2357	2359	2361	rBV	209	126	0.01%	0.002%
52	9.021	2387	2389	2392	rVB	326	182	0.02%	0.003%
53	9.041	2392	2395	2397	rBV	175	118	0.01%	0.002%
54	9.179	2435	2438	2441	rBV	158	110	0.01%	0.002%
55	9.262	2462	2464	2466	rBV	222	116	0.01%	0.002%
56	9.414	2497	2511	2530	rBV	449306	745209	85.20%	10.980%
57	9.568	2556	2559	2562	rBV	533	472	0.05%	0.007%
58	9.697	2591	2599	2607	rVB4	3334	4827	0.55%	0.071%
59	9.738	2607	2612	2613	rBV2	527	464	0.05%	0.007%
60	9.873	2652	2654	2658	rBV	168	95	0.01%	0.001%
61	9.954	2677	2679	2681	rBV	179	111	0.01%	0.002%
62	10.098	2718	2724	2738	rVB6	2610	4081	0.47%	0.060%
63	10.250	2769	2771	2774	rBV2	271	140	0.02%	0.002%
64	10.372	2807	2809	2813	rBV	235	134	0.02%	0.002%
65	10.430	2823	2827	2829	rBV	199	146	0.02%	0.002%
66	10.507	2850	2851	2855	rVB	403	136	0.02%	0.002%
67	10.639	2887	2892	2901	rBV3	764	824	0.09%	0.012%
68	10.751	2915	2927	2945	rBV	280692	458077	52.37%	6.749%
69	10.864	2960	2962	2964	rBV	243	111	0.01%	0.002%
70	10.912	2974	2977	2978	rBV	356	205	0.02%	0.003%
71	11.114	3033	3040	3047	rVB5	1611	2315	0.26%	0.034%
72	11.198	3063	3066	3067	rBV5	231	111	0.01%	0.002%
73	11.224	3071	3074	3077	rVB	211	126	0.01%	0.002%
74	11.311	3099	3101	3105	rVB2	390	226	0.03%	0.003%
75	11.375	3119	3121	3126	rVB	380	214	0.02%	0.003%
76	11.410	3130	3132	3133	rBV	370	151	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
 Data File : VU053514.D
 Acq On : 03 Apr 2023 12:54
 Operator : JC/MD
 Sample : 02121-07ME 5X
 Misc : 5.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C1180ME

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\SFAMULM033123WMA.M
 Title : VOC Analysis

77	11.741	3230	3235	3238	rBV3	789	875	0.10%	0.013%
78	11.806	3243	3255	3281	rVV	548286	874703	100.00%	12.888%
79	12.098	3344	3346	3348	rBV	324	173	0.02%	0.003%
80	12.188	3361	3374	3393	rBV	449823	727669	83.19%	10.722%
81	12.323	3410	3416	3424	rVB7	3735	5758	0.66%	0.085%
82	12.356	3424	3426	3428	rBV2	217	97	0.01%	0.001%
83	12.520	3472	3477	3478	rBV	333	278	0.03%	0.004%
84	12.590	3497	3499	3503	rBV2	394	227	0.03%	0.003%
85	12.687	3528	3529	3530	rBV2	299	86	0.01%	0.001%
86	12.931	3603	3605	3611	rVB4	430	309	0.04%	0.005%
87	13.005	3623	3628	3632	rVB5	669	677	0.08%	0.010%
88	13.028	3632	3635	3638	rBV2	551	386	0.04%	0.006%
89	13.044	3638	3640	3644	rVB3	827	605	0.07%	0.009%
90	13.217	3691	3694	3702	rVB2	602	771	0.09%	0.011%
91	13.249	3702	3704	3707	rBV	273	153	0.02%	0.002%
92	13.317	3723	3725	3728	rVB	533	216	0.02%	0.003%
93	13.352	3728	3736	3741	rVB4	569	728	0.08%	0.011%
94	13.375	3741	3743	3746	rBV	341	213	0.02%	0.003%
95	13.426	3752	3759	3768	rVB3	6784	9944	1.14%	0.147%
96	13.780	3867	3869	3871	rBV	415	196	0.02%	0.003%
97	13.838	3882	3887	3890	rBV4	1296	1305	0.15%	0.019%
98	14.330	4033	4040	4042	rBV3	1304	1405	0.16%	0.021%
99	14.446	4070	4076	4085	rVB3	10387	14069	1.61%	0.207%
100	14.523	4098	4100	4105	rBV4	709	511	0.06%	0.008%

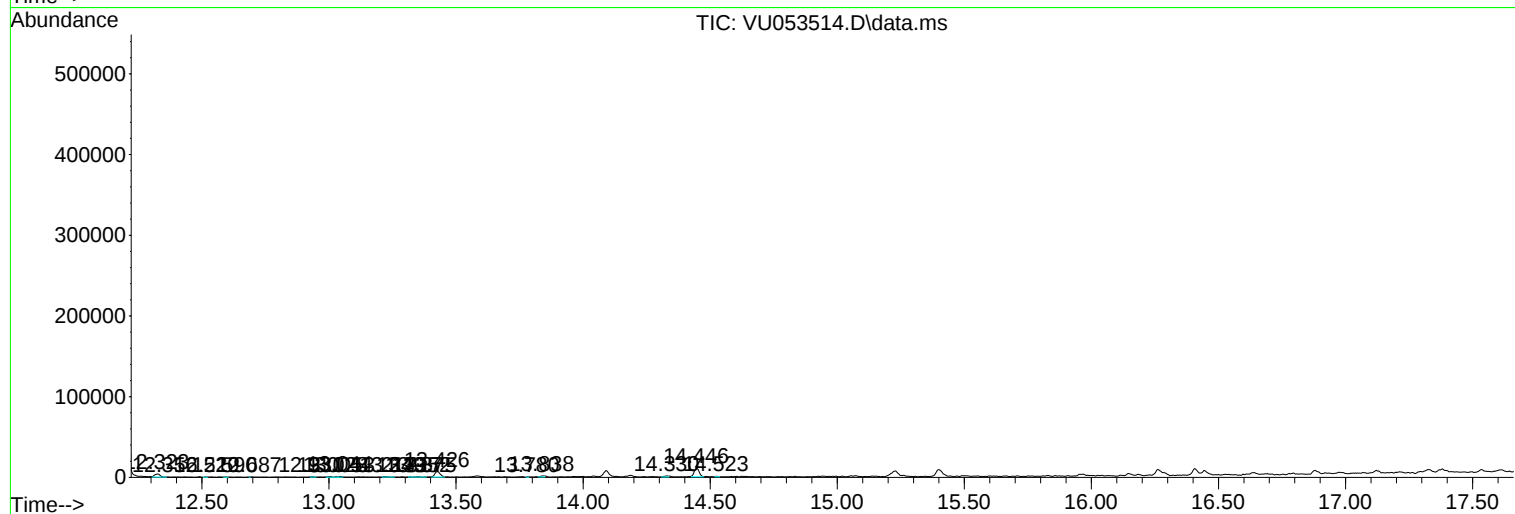
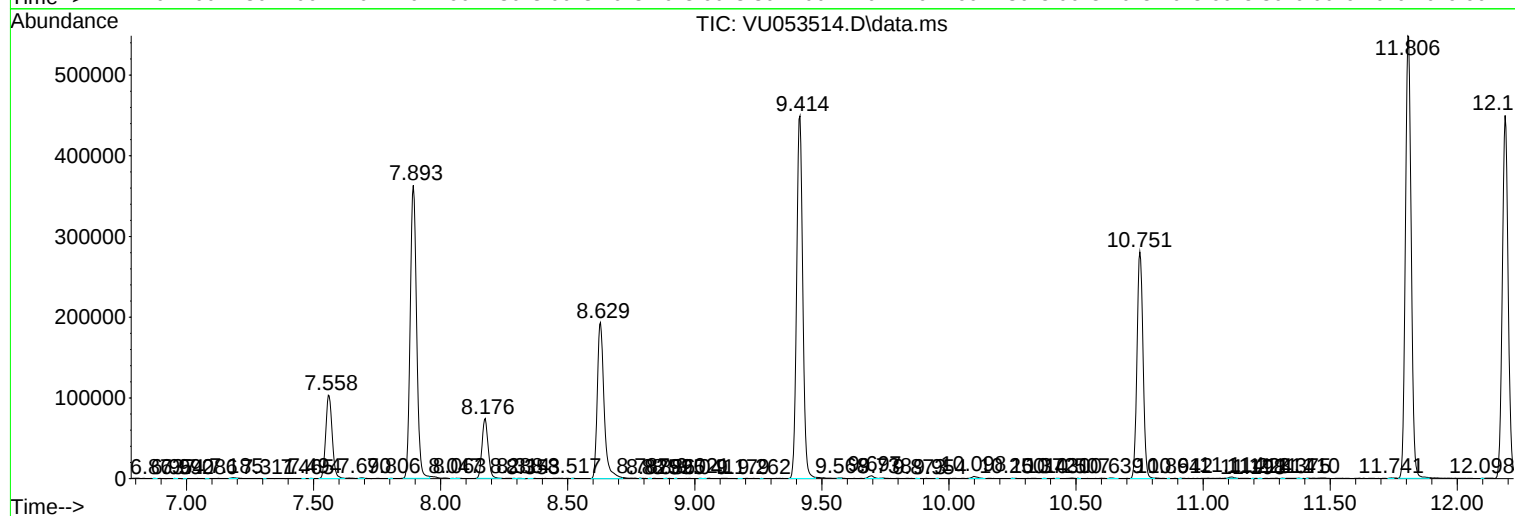
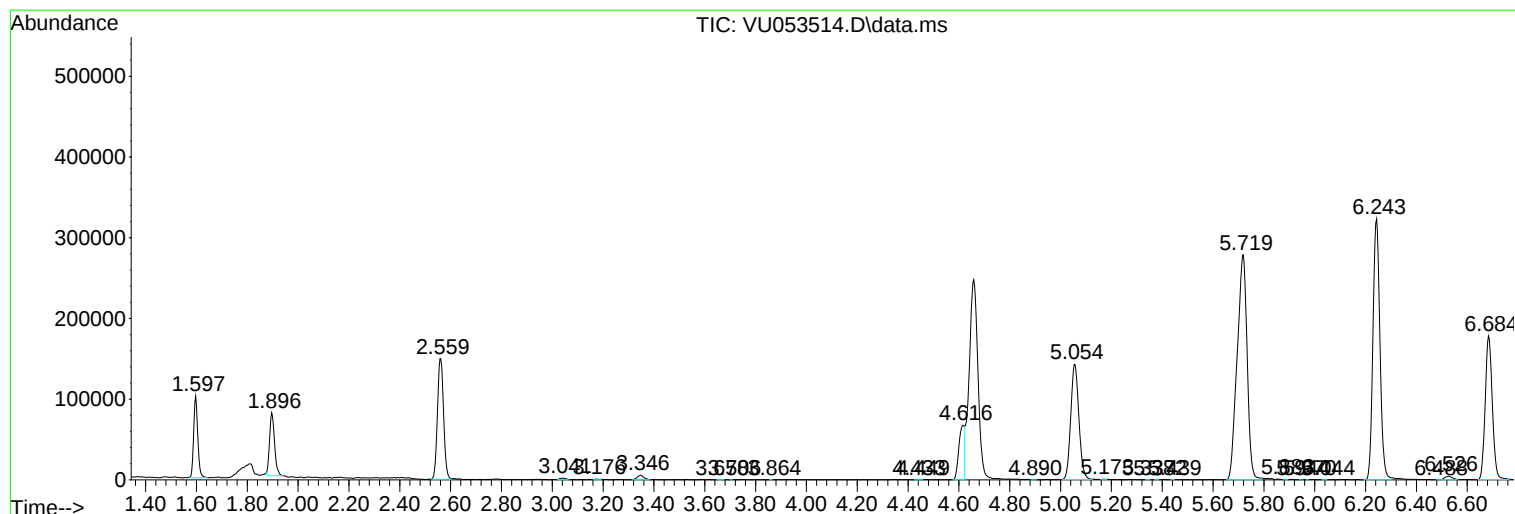
Sum of corrected areas: 6787000

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053514.D
Acq On : 03 Apr 2023 12:54
Operator : JC/MD
Sample : 02121-07ME 5X
Misc : 5.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1180ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU040323\
Data File : VU053514.D
Acq On : 03 Apr 2023 12:54
Operator : JC/MD
Sample : 02121-07ME 5X
Misc : 5.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1180ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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\VU040323\
Data File : VU053514.D
Acq On : 03 Apr 2023 12:54
Operator : JC/MD
Sample : 02121-07ME 5X
Misc : 5.46g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C1180ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.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
------------------	----	---------	-------	----------	---	----	------	------