

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050223\
 Data File : VU054048.D
 Acq On : 02 May 2023 16:11
 Operator : JC/MD
 Sample : 02564-03ME
 Misc : 5.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCE5ME

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\SFAMULM042923WMA.M
 Title : VOC Analysis

Signal : TIC: VU054048.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	99	rBV	65149	97366	11.83%	1.475%
2	1.903	170	175	192	rBV	36176	63342	7.70%	0.960%
3	2.549	363	376	390	rBV	166085	268997	32.69%	4.076%
4	2.732	431	433	437	rBV2	290	211	0.03%	0.003%
5	3.041	518	529	545	rBV2	4897	10815	1.31%	0.164%
6	3.166	566	568	576	rVB3	268	257	0.03%	0.004%
7	3.420	644	647	652	rVV2	192	196	0.02%	0.003%
8	3.459	655	659	662	rBV2	212	192	0.02%	0.003%
9	3.478	662	665	670	rVB2	232	244	0.03%	0.004%
10	3.510	670	675	678	rBV2	185	192	0.02%	0.003%
11	3.546	682	686	690	rBV2	145	166	0.02%	0.003%
12	3.768	752	755	757	rBV2	301	229	0.03%	0.003%
13	3.803	763	766	767	rBV	212	144	0.02%	0.002%
14	3.964	814	816	818	rBV	170	121	0.01%	0.002%
15	4.076	848	851	853	rBV	226	144	0.02%	0.002%
16	4.150	868	874	877	rBV2	291	312	0.04%	0.005%
17	4.420	954	958	962	rBV	295	310	0.04%	0.005%
18	4.510	983	986	989	rBV2	185	129	0.02%	0.002%
19	4.575	1001	1006	1010	rBV3	266	220	0.03%	0.003%
20	4.636	1013	1025	1050	rBV2	39498	131191	15.94%	1.988%
21	4.983	1130	1133	1136	rVB	265	171	0.02%	0.003%
22	5.057	1139	1156	1184	rVV	134212	324748	39.47%	4.921%
23	5.214	1198	1205	1207	rBV3	823	901	0.11%	0.014%
24	5.317	1231	1237	1240	rBV	259	283	0.03%	0.004%
25	5.456	1275	1280	1283	rVB	279	280	0.03%	0.004%
26	5.475	1283	1286	1288	rBV	254	188	0.02%	0.003%
27	5.517	1295	1299	1303	rBV2	195	195	0.02%	0.003%
28	5.549	1305	1309	1310	rBV	239	170	0.02%	0.003%
29	5.616	1324	1330	1333	rBV2	217	279	0.03%	0.004%
30	5.716	1341	1361	1389	rBV2	311915	822804	100.00%	12.469%
31	5.941	1428	1431	1435	rBV	235	217	0.03%	0.003%
32	5.976	1435	1442	1450	rBV4	1488	2487	0.30%	0.038%
33	6.050	1462	1465	1466	rBV	308	183	0.02%	0.003%
34	6.118	1483	1486	1489	rVV2	382	267	0.03%	0.004%
35	6.157	1494	1498	1500	rBV	181	138	0.02%	0.002%
36	6.243	1511	1525	1555	rBV	324785	653155	79.38%	9.898%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050223\
 Data File : VU054048.D
 Acq On : 02 May 2023 16:11
 Operator : JC/MD
 Sample : 02564-03ME
 Misc : 5.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCE5ME

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\SFAMULM042923WMA.M
 Title : VOC Analysis

37	6.465	1590	1594	1598	rBV2	294	293	0.04%	0.004%
38	6.530	1604	1614	1623	rBV5	3502	6764	0.82%	0.102%
39	6.603	1629	1637	1646	rBV3	1953	3650	0.44%	0.055%
40	6.684	1649	1662	1683	rBV	183233	363785	44.21%	5.513%
41	6.787	1691	1694	1696	rBV2	198	109	0.01%	0.002%
42	6.870	1716	1720	1726	rBV2	176	207	0.03%	0.003%
43	6.899	1726	1729	1732	rBV	153	122	0.01%	0.002%
44	6.919	1732	1735	1738	rBV	192	169	0.02%	0.003%
45	7.009	1758	1763	1765	rBV2	176	189	0.02%	0.003%
46	7.031	1767	1770	1776	rVV2	213	285	0.03%	0.004%
47	7.105	1789	1793	1796	rBV2	318	282	0.03%	0.004%
48	7.160	1806	1810	1814	rBV	165	181	0.02%	0.003%
49	7.195	1814	1821	1822	rBV3	1778	1695	0.21%	0.026%
50	7.282	1845	1848	1850	rBV2	185	104	0.01%	0.002%
51	7.295	1850	1852	1855	rBV2	168	120	0.01%	0.002%
52	7.311	1855	1857	1859	rVV2	227	115	0.01%	0.002%
53	7.385	1876	1880	1881	rBV	184	152	0.02%	0.002%
54	7.414	1887	1889	1894	rVB2	243	191	0.02%	0.003%
55	7.443	1894	1898	1899	rBV	216	160	0.02%	0.002%
56	7.478	1906	1909	1911	rBV	148	126	0.02%	0.002%
57	7.562	1922	1935	1959	rBV2	96775	182734	22.21%	2.769%
58	7.687	1970	1974	1976	rBV2	207	212	0.03%	0.003%
59	7.729	1984	1987	1989	rVB2	446	266	0.03%	0.004%
60	7.748	1989	1993	1997	rBV2	249	279	0.03%	0.004%
61	7.893	2025	2038	2060	rBV	360569	653983	79.48%	9.910%
62	8.179	2115	2127	2155	rBV	61747	125565	15.26%	1.903%
63	8.327	2169	2173	2175	rBV	154	140	0.02%	0.002%
64	8.420	2200	2202	2205	rBV2	250	169	0.02%	0.003%
65	8.472	2210	2218	2221	rBV2	464	754	0.09%	0.011%
66	8.529	2232	2236	2237	rBV	371	293	0.04%	0.004%
67	8.603	2256	2259	2260	rBV	218	126	0.02%	0.002%
68	8.658	2260	2276	2304	rVV	145304	322186	39.16%	4.882%
69	8.861	2336	2339	2342	rBV2	168	144	0.02%	0.002%
70	8.880	2342	2345	2350	rVV2	281	241	0.03%	0.004%
71	9.269	2462	2466	2468	rBV2	175	166	0.02%	0.003%
72	9.417	2498	2512	2545	rBV	409285	776789	94.41%	11.771%
73	9.697	2591	2599	2611	rVB5	2197	4468	0.54%	0.068%
74	9.745	2611	2614	2617	rVB2	189	128	0.02%	0.002%
75	9.780	2621	2625	2626	rBV	191	158	0.02%	0.002%
76	9.819	2635	2637	2640	rBV	181	132	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050223\
 Data File : VU054048.D
 Acq On : 02 May 2023 16:11
 Operator : JC/MD
 Sample : 02564-03ME
 Misc : 5.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCCE5ME

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\SFAMULM042923WMA.M
 Title : VOC Analysis

77	9.957	2677	2680	2683	rVB2	328	217	0.03%	0.003%
78	9.986	2683	2689	2692	rBV2	267	342	0.04%	0.005%
79	10.108	2721	2727	2729	rBV3	733	779	0.09%	0.012%
80	10.179	2747	2749	2751	rBV	197	137	0.02%	0.002%
81	10.217	2758	2761	2764	rVB2	221	157	0.02%	0.002%
82	10.478	2840	2842	2845	rBV2	330	245	0.03%	0.004%
83	10.517	2852	2854	2857	rVB2	185	107	0.01%	0.002%
84	10.542	2857	2862	2863	rBV	171	153	0.02%	0.002%
85	10.613	2881	2884	2886	rBV4	349	246	0.03%	0.004%
86	10.761	2915	2930	2946	rBV	235164	383169	46.57%	5.806%
87	11.118	3036	3041	3044	rVB4	1435	1431	0.17%	0.022%
88	11.243	3075	3080	3086	rVB2	226	274	0.03%	0.004%
89	11.314	3100	3102	3104	rVB	276	127	0.02%	0.002%
90	11.333	3104	3108	3111	rBV2	279	275	0.03%	0.004%
91	11.398	3125	3128	3131	rBV3	309	240	0.03%	0.004%
92	11.468	3147	3150	3158	rVB3	437	533	0.06%	0.008%
93	11.536	3167	3171	3177	rBV2	468	543	0.07%	0.008%
94	11.706	3222	3224	3226	rBV	219	125	0.02%	0.002%
95	11.745	3233	3236	3238	rBV	461	352	0.04%	0.005%
96	11.812	3244	3257	3277	rBV	490372	773385	93.99%	11.720%
97	12.015	3317	3320	3323	rBV	287	197	0.02%	0.003%
98	12.098	3343	3346	3348	rBV	255	179	0.02%	0.003%
99	12.192	3363	3375	3398	rBV	376465	606816	73.75%	9.196%
100	12.922	3600	3602	3606	rBV2	267	148	0.02%	0.002%

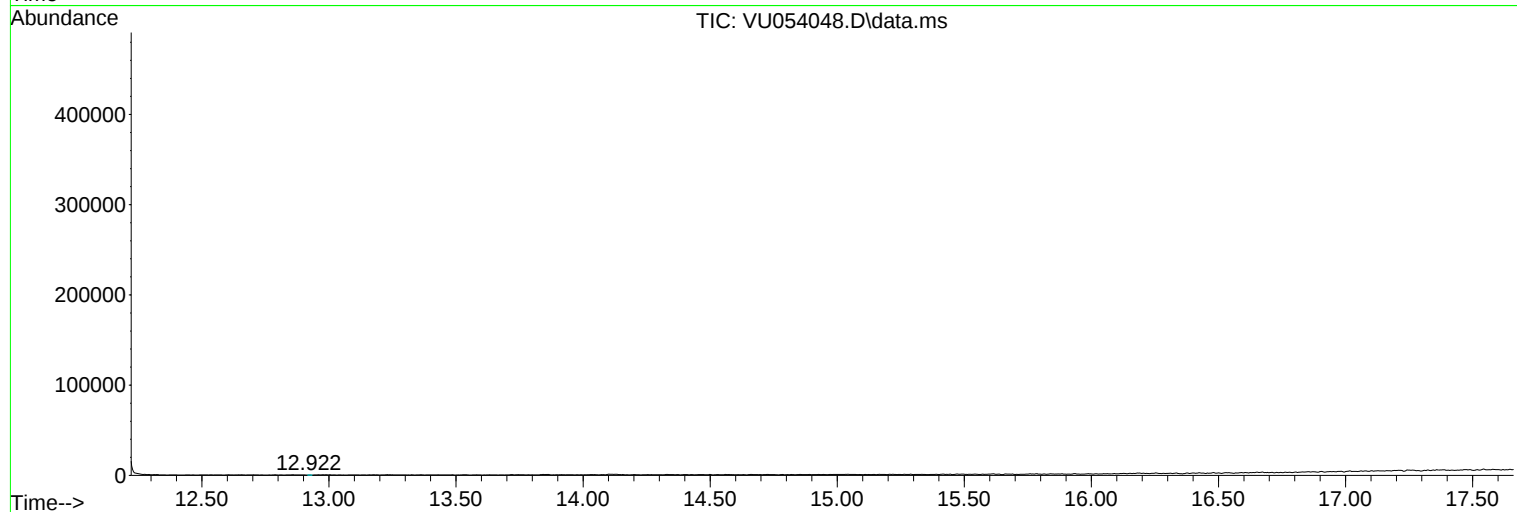
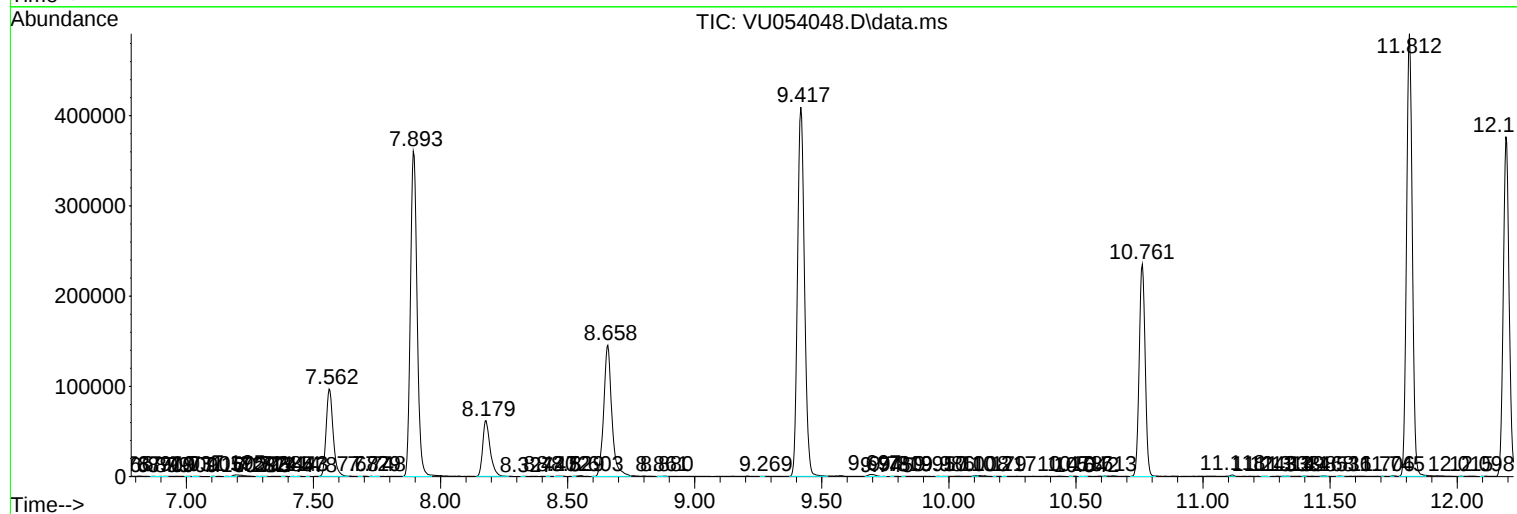
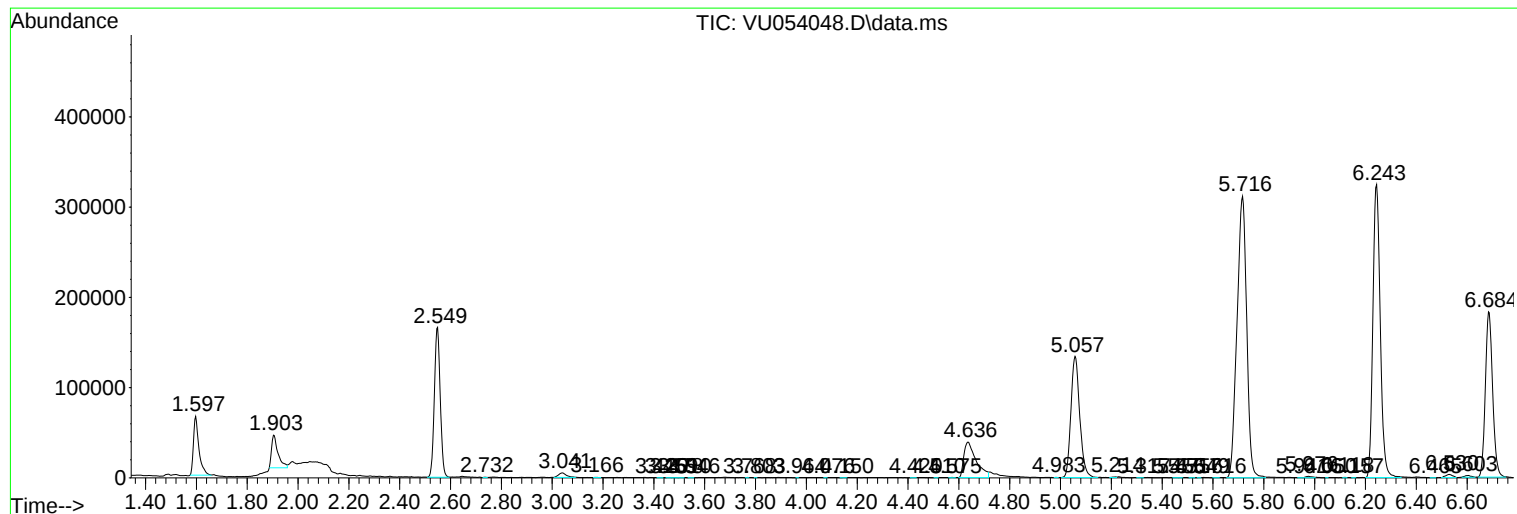
Sum of corrected areas: 6599053

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050223\
Data File : VU054048.D
Acq On : 02 May 2023 16:11
Operator : JC/MD
Sample : 02564-03ME
Misc : 5.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCCE5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050223\
Data File : VU054048.D
Acq On : 02 May 2023 16:11
Operator : JC/MD
Sample : 02564-03ME
Misc : 5.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCCE5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.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\VU050223\
Data File : VU054048.D
Acq On : 02 May 2023 16:11
Operator : JC/MD
Sample : 02564-03ME
Misc : 5.72g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DCCE5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042923WMA.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