

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071422\
 Data File : VU049714.D
 Acq On : 14 Jul 2022 13:07
 Operator : SY/MD
 Sample : N3678-01ME
 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B20ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049714.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	40	44	49	rVB2	3031	2684	0.31%	0.038%
2	1.510	49	53	58	rBV4	2260	3000	0.35%	0.043%
3	1.594	72	79	86	rBV	48858	67082	7.81%	0.953%
4	1.858	126	161	162	rBV2	25372	71071	8.28%	1.009%
5	1.880	164	168	179	rVV	29727	42812	4.99%	0.608%
6	2.366	317	319	324	rBV3	636	472	0.05%	0.007%
7	2.443	339	343	348	rBV3	498	629	0.07%	0.009%
8	2.526	358	369	383	rBV	151383	242008	28.18%	3.437%
9	2.629	397	401	403	rBV3	442	374	0.04%	0.005%
10	2.649	403	407	418	rVB6	1153	2029	0.24%	0.029%
11	2.797	449	453	455	rBV	226	164	0.02%	0.002%
12	2.951	496	501	503	rBV3	503	477	0.06%	0.007%
13	3.028	518	525	539	rVB3	2618	4736	0.55%	0.067%
14	3.176	556	571	588	rBV	22259	51905	6.04%	0.737%
15	3.330	615	619	623	rBV	302	220	0.03%	0.003%
16	3.359	623	628	634	rVB2	191	211	0.02%	0.003%
17	3.388	634	637	640	rBV	262	179	0.02%	0.003%
18	3.501	667	672	677	rVV	303	322	0.04%	0.005%
19	3.526	677	680	686	rVB2	203	169	0.02%	0.002%
20	3.610	702	706	709	rBV2	206	188	0.02%	0.003%
21	3.681	723	728	729	rBV	208	183	0.02%	0.003%
22	3.928	801	805	808	rBV	330	238	0.03%	0.003%
23	4.150	869	874	877	rBV2	180	177	0.02%	0.003%
24	4.169	877	880	885	rVB	327	307	0.04%	0.004%
25	4.214	885	894	900	rBV2	310	679	0.08%	0.010%
26	4.263	906	909	914	rBV2	294	281	0.03%	0.004%
27	4.304	920	922	929	rVV2	241	221	0.03%	0.003%
28	4.481	973	977	983	rVB2	287	232	0.03%	0.003%
29	4.639	1007	1026	1065	rBV	82578	279194	32.51%	3.965%
30	4.986	1131	1134	1138	rBV2	364	228	0.03%	0.003%
31	5.060	1138	1157	1179	rBV	154489	357099	41.58%	5.071%
32	5.288	1221	1228	1236	rVB3	763	1356	0.16%	0.019%
33	5.353	1245	1248	1250	rBV2	349	222	0.03%	0.003%
34	5.372	1250	1254	1259	rVB2	459	568	0.07%	0.008%
35	5.510	1289	1297	1299	rBV2	182	279	0.03%	0.004%
36	5.716	1341	1361	1386	rBV3	331793	858762	100.00%	12.195%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071422\
 Data File : VU049714.D
 Acq On : 14 Jul 2022 13:07
 Operator : SY/MD
 Sample : N3678-01ME
 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B20ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

37	5.809	1386	1390	1398	rVB5	470	505	0.06%	0.007%
38	5.980	1432	1443	1457	rBV5	7796	18432	2.15%	0.262%
39	6.243	1510	1525	1549	rBV	275585	545270	63.49%	7.743%
40	6.343	1553	1556	1560	rVB3	318	240	0.03%	0.003%
41	6.427	1573	1582	1588	rVB2	293	479	0.06%	0.007%
42	6.523	1604	1612	1624	rVV8	4462	8683	1.01%	0.123%
43	6.603	1626	1637	1649	rVV4	3619	7888	0.92%	0.112%
44	6.687	1649	1663	1690	rVB	203089	417752	48.65%	5.932%
45	6.803	1694	1699	1701	rBV4	309	260	0.03%	0.004%
46	6.999	1756	1760	1766	rBV2	179	176	0.02%	0.002%
47	7.192	1812	1820	1823	rBV6	2463	3922	0.46%	0.056%
48	7.311	1852	1857	1860	rVB3	345	272	0.03%	0.004%
49	7.565	1923	1936	1955	rBV	95659	179894	20.95%	2.555%
50	7.693	1969	1976	1982	rBV4	1508	1998	0.23%	0.028%
51	7.780	1998	2003	2004	rBV2	322	221	0.03%	0.003%
52	7.896	2025	2039	2059	rBV	356855	633859	73.81%	9.001%
53	7.992	2059	2069	2084	rVV4	4445	10380	1.21%	0.147%
54	8.047	2084	2086	2089	rVB2	360	168	0.02%	0.002%
55	8.070	2089	2093	2096	rBV2	352	276	0.03%	0.004%
56	8.182	2114	2128	2148	rVV	61213	118716	13.82%	1.686%
57	8.346	2177	2179	2181	rBV	512	273	0.03%	0.004%
58	8.449	2208	2211	2214	rBV2	289	170	0.02%	0.002%
59	8.584	2249	2253	2259	rBV2	177	183	0.02%	0.003%
60	8.658	2259	2276	2305	rBV	248349	617085	71.86%	8.763%
61	8.796	2312	2319	2331	rVB6	2617	4708	0.55%	0.067%
62	8.931	2357	2361	2364	rBV3	648	534	0.06%	0.008%
63	9.070	2399	2404	2406	rBV2	212	200	0.02%	0.003%
64	9.105	2411	2415	2418	rBV2	232	218	0.03%	0.003%
65	9.349	2488	2491	2494	rBV	277	203	0.02%	0.003%
66	9.420	2499	2513	2533	rBV	362356	673706	78.45%	9.567%
67	9.545	2549	2552	2556	rVB2	303	259	0.03%	0.004%
68	9.571	2556	2560	2563	rBV	470	335	0.04%	0.005%
69	9.780	2622	2625	2628	rBV2	340	297	0.03%	0.004%
70	9.889	2656	2659	2663	rVB2	293	233	0.03%	0.003%
71	9.944	2672	2676	2679	rBV	262	175	0.02%	0.002%
72	10.047	2704	2708	2711	rBV2	186	181	0.02%	0.003%
73	10.279	2775	2780	2784	rBV2	249	215	0.03%	0.003%
74	10.346	2798	2801	2803	rBV	250	192	0.02%	0.003%
75	10.597	2877	2879	2883	rVB3	298	197	0.02%	0.003%
76	10.623	2883	2887	2891	rBV4	650	505	0.06%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071422\
 Data File : VU049714.D
 Acq On : 14 Jul 2022 13:07
 Operator : SY/MD
 Sample : N3678-01ME
 Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B20ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

77	10.648	2891	2895	2896	rBV3	614	436	0.05%	0.006%
78	10.764	2917	2931	2950	rVV	323508	529260	61.63%	7.516%
79	10.844	2953	2956	2957	rVV	262	169	0.02%	0.002%
80	10.906	2970	2975	2979	rBV2	375	355	0.04%	0.005%
81	11.114	3035	3040	3045	rVB2	1497	1588	0.18%	0.023%
82	11.314	3098	3102	3107	rVB3	366	419	0.05%	0.006%
83	11.369	3116	3119	3121	rBV2	268	177	0.02%	0.003%
84	11.815	3245	3258	3273	rBV	407364	633312	73.75%	8.994%
85	11.918	3288	3290	3296	rVB	481	332	0.04%	0.005%
86	12.044	3326	3329	3333	rBV	252	233	0.03%	0.003%
87	12.195	3364	3376	3392	rVV	399001	630381	73.41%	8.952%
88	12.397	3437	3439	3441	rBV2	252	173	0.02%	0.002%
89	12.433	3447	3450	3456	rVB2	298	269	0.03%	0.004%
90	12.770	3549	3555	3557	rBV2	360	318	0.04%	0.005%
91	12.938	3601	3607	3614	rVB2	351	402	0.05%	0.006%
92	13.356	3731	3737	3743	rBV2	379	668	0.08%	0.009%
93	13.606	3812	3815	3818	rBV2	555	453	0.05%	0.006%
94	13.819	3878	3881	3885	rBV2	281	285	0.03%	0.004%
95	14.407	4060	4064	4066	rBV3	504	414	0.05%	0.006%
96	14.658	4138	4142	4147	rBV2	533	501	0.06%	0.007%
97	15.040	4259	4261	4268	rVB3	357	306	0.04%	0.004%
98	15.777	4487	4490	4495	rVB2	802	675	0.08%	0.010%
99	16.249	4635	4637	4640	rBV3	632	351	0.04%	0.005%
100	16.368	4671	4674	4675	rBV3	658	377	0.04%	0.005%

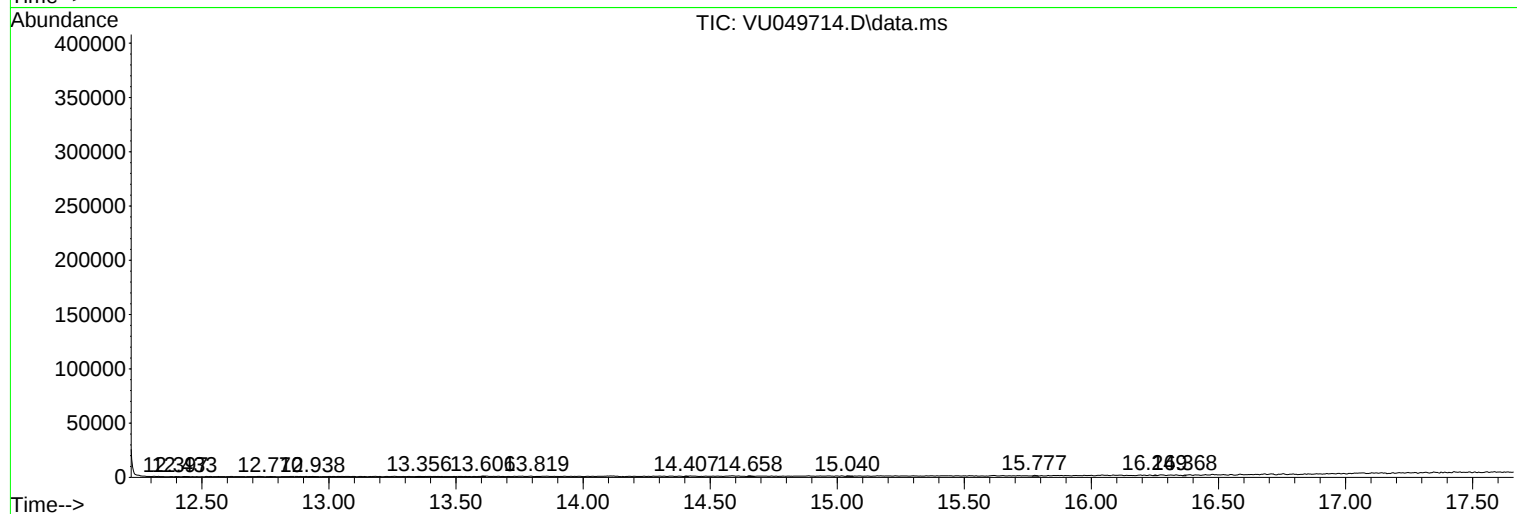
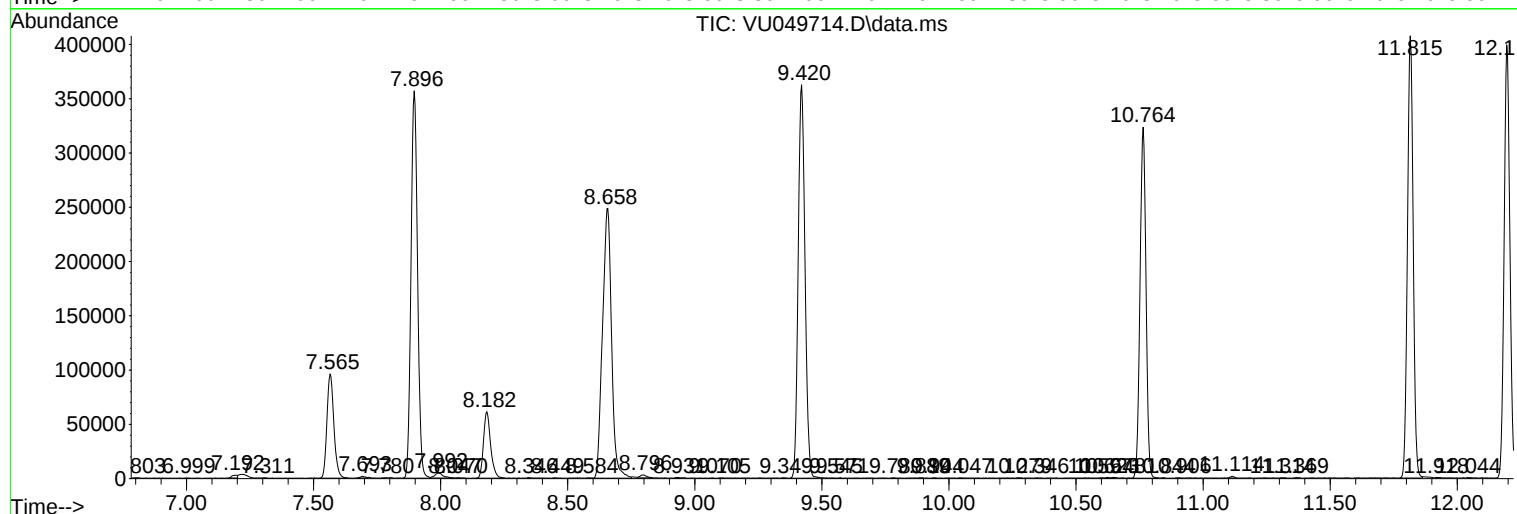
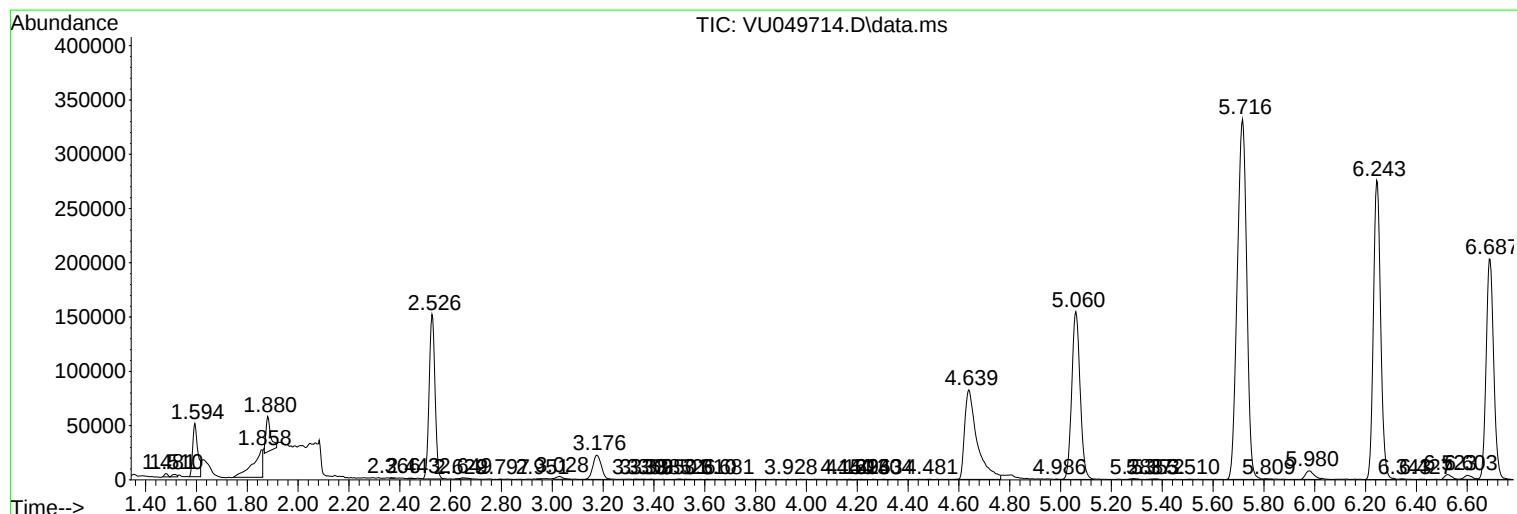
Sum of corrected areas: 7041872

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071422\
Data File : VU049714.D
Acq On : 14 Jul 2022 13:07
Operator : SY/MD
Sample : N3678-01ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B20ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071422\
Data File : VU049714.D
Acq On : 14 Jul 2022 13:07
Operator : SY/MD
Sample : N3678-01ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B20ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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\VU071422\
Data File : VU049714.D
Acq On : 14 Jul 2022 13:07
Operator : SY/MD
Sample : N3678-01ME
Misc : 5.99g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B20ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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
------------------	----	---------	-------	----------	---	----	------	------