

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049801.D
 Acq On : 20 Jul 2022 12:58
 Operator : SY/MD
 Sample : N3721-08ME
 Misc : 6.25g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5C28ME

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: VU049801.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	48	rVB4	2291	1980	0.28%	0.034%
2	1.510	48	53	57	rBV	2374	2603	0.36%	0.045%
3	1.594	71	79	85	rBV	48445	64224	8.98%	1.103%
4	1.851	125	159	161	rBV4	35348	95575	13.36%	1.641%
5	1.871	162	165	178	rVB	28523	44194	6.18%	0.759%
6	2.321	301	305	309	rBV5	835	790	0.11%	0.014%
7	2.523	356	368	385	rBV	132760	215224	30.08%	3.696%
8	2.649	398	407	416	rBV3	1468	2982	0.42%	0.051%
9	2.925	489	493	496	rBV	329	261	0.04%	0.004%
10	2.951	496	501	502	rVV3	570	462	0.06%	0.008%
11	2.964	502	505	509	rVV3	711	640	0.09%	0.011%
12	3.025	512	524	538	rBV6	4705	9312	1.30%	0.160%
13	3.176	558	571	592	rBV	7992	18444	2.58%	0.317%
14	3.269	597	600	608	rVB2	231	312	0.04%	0.005%
15	3.433	648	651	657	rVB2	286	332	0.05%	0.006%
16	3.465	657	661	667	rBV2	271	397	0.06%	0.007%
17	3.514	672	676	680	rVB2	263	265	0.04%	0.005%
18	3.665	719	723	728	rBV3	651	567	0.08%	0.010%
19	3.758	748	752	756	rVB2	208	208	0.03%	0.004%
20	3.796	761	764	770	rVB	175	162	0.02%	0.003%
21	3.899	792	796	800	rVB	259	196	0.03%	0.003%
22	4.395	947	950	954	rBV2	205	182	0.03%	0.003%
23	4.468	967	973	979	rBV2	216	312	0.04%	0.005%
24	4.523	986	990	993	rBV	232	162	0.02%	0.003%
25	4.546	993	997	1000	rVB2	218	191	0.03%	0.003%
26	4.636	1013	1025	1057	rBV	66143	204182	28.54%	3.506%
27	4.854	1090	1093	1098	rBV3	203	220	0.03%	0.004%
28	4.970	1122	1129	1132	rBV3	363	450	0.06%	0.008%
29	5.057	1140	1156	1184	rBV	123802	284871	39.81%	4.892%
30	5.208	1199	1203	1204	rBV	358	220	0.03%	0.004%
31	5.250	1211	1216	1220	rBV2	161	241	0.03%	0.004%
32	5.282	1220	1226	1228	rBV	581	614	0.09%	0.011%
33	5.375	1252	1255	1257	rVB	307	169	0.02%	0.003%
34	5.404	1257	1264	1265	rBV	171	192	0.03%	0.003%
35	5.523	1295	1301	1303	rBV	176	160	0.02%	0.003%
36	5.716	1341	1361	1382	rVV2	279317	715528	100.00%	12.288%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049801.D
 Acq On : 20 Jul 2022 12:58
 Operator : SY/MD
 Sample : N3721-08ME
 Misc : 6.25g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5C28ME

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	5.980	1430	1443	1461	rVV5	7318	17556	2.45%	0.301%
38	6.086	1468	1476	1478	rBV2	185	209	0.03%	0.004%
39	6.163	1495	1500	1503	rBV2	229	256	0.04%	0.004%
40	6.243	1512	1525	1546	rVV	249934	487603	68.15%	8.374%
41	6.356	1558	1560	1564	rVB2	334	166	0.02%	0.003%
42	6.526	1600	1613	1622	rBV7	3016	5779	0.81%	0.099%
43	6.600	1626	1636	1649	rVV5	3457	7482	1.05%	0.128%
44	6.687	1649	1663	1684	rVB	167110	335369	46.87%	5.759%
45	6.761	1684	1686	1691	rVB3	267	155	0.02%	0.003%
46	7.221	1810	1829	1841	rVV9	2998	9577	1.34%	0.164%
47	7.266	1841	1843	1848	rVV2	352	243	0.03%	0.004%
48	7.311	1852	1857	1861	rVV3	300	315	0.04%	0.005%
49	7.430	1889	1894	1898	rBV2	450	449	0.06%	0.008%
50	7.565	1924	1936	1958	rBV	81145	152606	21.33%	2.621%
51	7.697	1974	1977	1979	rVB2	524	298	0.04%	0.005%
52	7.745	1988	1992	1997	rBV2	241	189	0.03%	0.003%
53	7.896	2023	2039	2059	rBV	292796	520328	72.72%	8.936%
54	7.989	2060	2068	2082	rVB4	4519	9369	1.31%	0.161%
55	8.057	2084	2089	2092	rBV3	290	253	0.04%	0.004%
56	8.182	2116	2128	2147	rBV2	52320	100329	14.02%	1.723%
57	8.250	2147	2149	2152	rVV2	377	224	0.03%	0.004%
58	8.314	2167	2169	2173	rVV	183	155	0.02%	0.003%
59	8.356	2173	2182	2187	rVB4	694	911	0.13%	0.016%
60	8.382	2187	2190	2196	rBV2	216	257	0.04%	0.004%
61	8.404	2196	2197	2202	rVB2	276	178	0.02%	0.003%
62	8.652	2258	2274	2306	rBV2	189040	467271	65.30%	8.024%
63	8.761	2306	2308	2310	rVV4	658	450	0.06%	0.008%
64	8.799	2313	2320	2330	rVB6	2200	3972	0.56%	0.068%
65	8.857	2336	2338	2343	rVB2	371	226	0.03%	0.004%
66	8.899	2343	2351	2356	rBV2	232	375	0.05%	0.006%
67	8.938	2359	2363	2366	rBV2	281	232	0.03%	0.004%
68	9.182	2436	2439	2443	rBV2	203	164	0.02%	0.003%
69	9.420	2499	2513	2531	rBV	328631	595872	83.28%	10.233%
70	9.574	2559	2561	2564	rVB	403	210	0.03%	0.004%
71	9.594	2564	2567	2571	rBV2	240	269	0.04%	0.005%
72	9.947	2673	2677	2680	rBV2	253	200	0.03%	0.003%
73	10.037	2702	2705	2708	rBV	233	155	0.02%	0.003%
74	10.066	2711	2714	2721	rVV2	149	201	0.03%	0.003%
75	10.205	2753	2757	2759	rBV	172	156	0.02%	0.003%
76	10.488	2841	2845	2849	rVB2	295	270	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049801.D
 Acq On : 20 Jul 2022 12:58
 Operator : SY/MD
 Sample : N3721-08ME
 Misc : 6.25g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5C28ME

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	10.655	2895	2897	2900	rVB2	440	219	0.03%	0.004%
78	10.761	2917	2930	2952	rBV	244677	405805	56.71%	6.969%
79	10.909	2973	2976	2979	rBV	225	154	0.02%	0.003%
80	10.928	2979	2982	2987	rVV2	248	241	0.03%	0.004%
81	11.069	3023	3026	3028	rBV2	243	175	0.02%	0.003%
82	11.095	3031	3034	3035	rVV2	239	156	0.02%	0.003%
83	11.118	3035	3041	3048	rVB5	1061	1473	0.21%	0.025%
84	11.433	3137	3139	3145	rBV2	178	156	0.02%	0.003%
85	11.600	3188	3191	3196	rBV2	235	229	0.03%	0.004%
86	11.815	3245	3258	3274	rBV	343040	554841	77.54%	9.528%
87	12.082	3339	3341	3346	rVB2	199	154	0.02%	0.003%
88	12.195	3364	3376	3396	rBV	287813	468108	65.42%	8.039%
89	12.375	3428	3432	3435	rBV2	317	317	0.04%	0.005%
90	12.722	3536	3540	3544	rBV2	216	214	0.03%	0.004%
91	12.764	3549	3553	3556	rBV2	324	302	0.04%	0.005%
92	12.889	3590	3592	3596	rBV	252	158	0.02%	0.003%
93	13.047	3638	3641	3642	rBV	257	163	0.02%	0.003%
94	13.346	3728	3734	3736	rBV2	376	380	0.05%	0.007%
95	13.709	3844	3847	3853	rBV2	284	292	0.04%	0.005%
96	14.301	4028	4031	4033	rBV2	318	185	0.03%	0.003%
97	14.365	4048	4051	4055	rVB2	268	208	0.03%	0.004%
98	14.388	4055	4058	4061	rBV3	342	212	0.03%	0.004%
99	14.574	4110	4116	4123	rVB3	1073	1510	0.21%	0.026%
100	15.960	4545	4547	4550	rBV	552	345	0.05%	0.006%

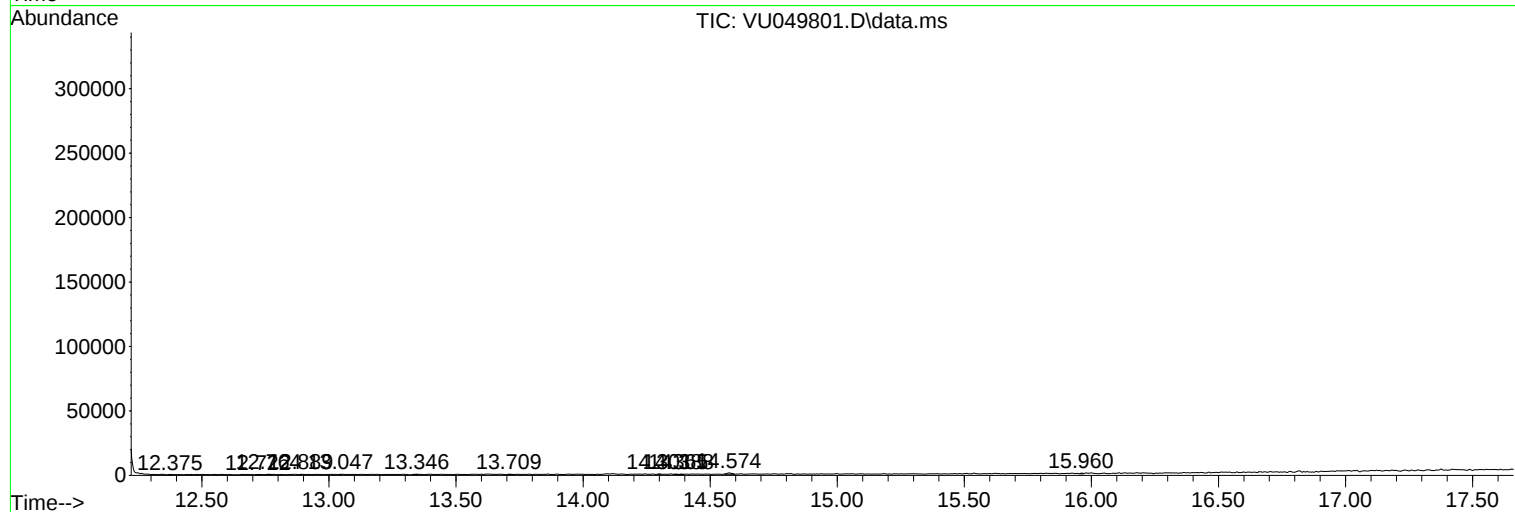
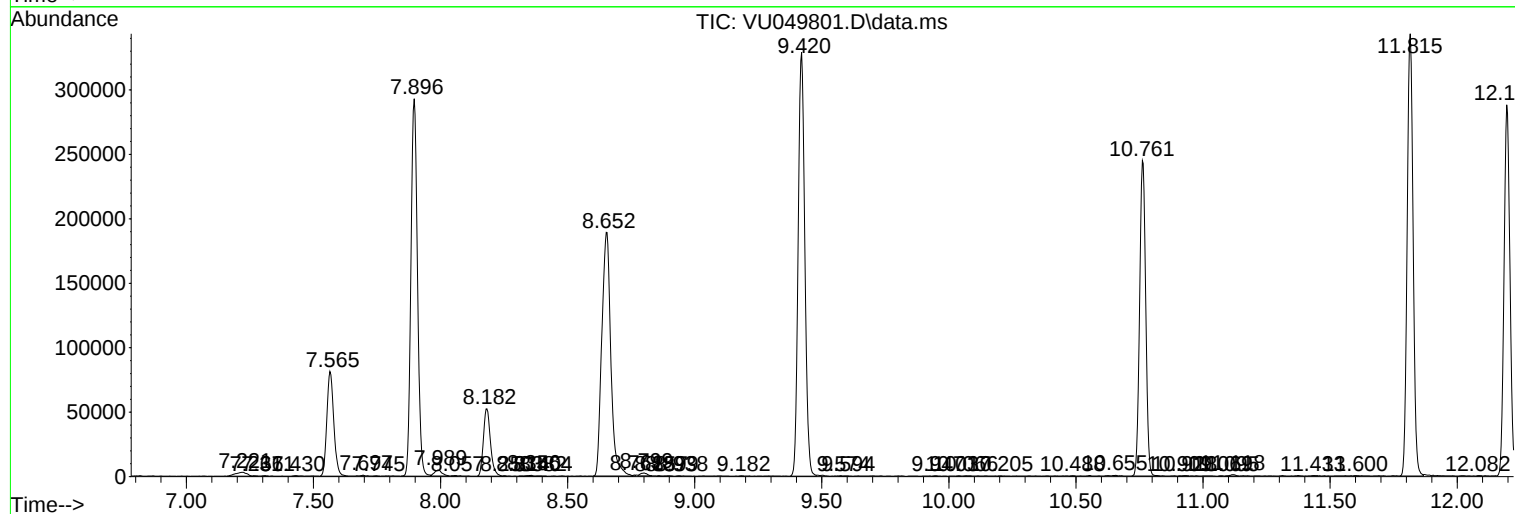
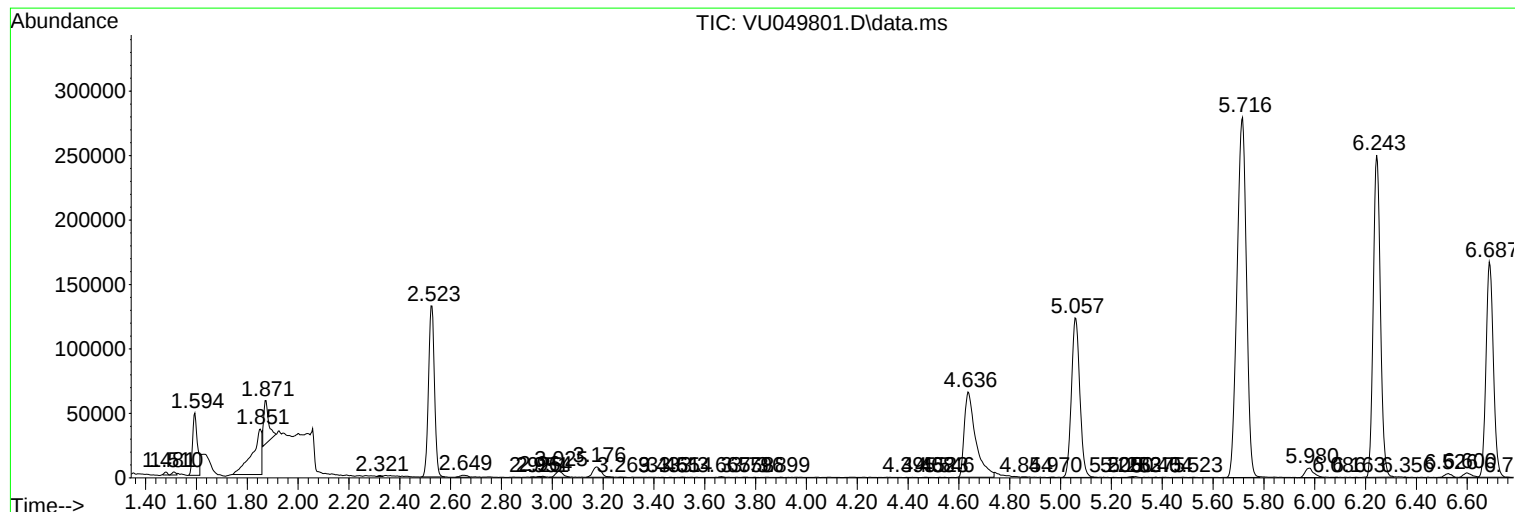
Sum of corrected areas: 5823100

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
Data File : VU049801.D
Acq On : 20 Jul 2022 12:58
Operator : SY/MD
Sample : N3721-08ME
Misc : 6.25g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5C28ME

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\VU072022\
Data File : VU049801.D
Acq On : 20 Jul 2022 12:58
Operator : SY/MD
Sample : N3721-08ME
Misc : 6.25g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5C28ME

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\VU072022\
Data File : VU049801.D
Acq On : 20 Jul 2022 12:58
Operator : SY/MD
Sample : N3721-08ME
Misc : 6.25g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5C28ME

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
------------------	----	---------	-------	----------	---	----	------	------