

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050505.D
 Acq On : 29 Aug 2022 23:52
 Operator : SY/MD
 Sample : N4344-19ME
 Misc : 5.85g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVR6ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050505.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.591	72	78	87	rBV	92207	126260	7.59%	1.076%
2	2.526	358	369	389	rVB	305089	492828	29.61%	4.199%
3	3.028	516	525	536	rBV2	7580	14897	0.90%	0.127%
4	3.121	551	554	556	rBV2	278	154	0.01%	0.001%
5	3.176	559	571	588	rBV	19446	53285	3.20%	0.454%
6	3.452	651	657	661	rBV4	457	574	0.03%	0.005%
7	3.491	666	669	673	rVB2	252	198	0.01%	0.002%
8	3.510	673	675	676	rBV	216	89	0.01%	0.001%
9	3.549	684	687	688	rBV	208	114	0.01%	0.001%
10	3.575	692	695	699	rVV	242	183	0.01%	0.002%
11	3.623	707	710	712	rBV	176	117	0.01%	0.001%
12	3.665	715	723	733	rBV5	763	1232	0.07%	0.010%
13	3.710	735	737	742	rVB	248	127	0.01%	0.001%
14	3.758	749	752	757	rBV	287	273	0.02%	0.002%
15	3.870	785	787	790	rBV	192	148	0.01%	0.001%
16	3.903	793	797	801	rBV2	181	182	0.01%	0.002%
17	3.925	801	804	808	rVV2	156	117	0.01%	0.001%
18	4.009	825	830	834	rBV2	220	261	0.02%	0.002%
19	4.166	875	879	881	rBV2	247	184	0.01%	0.002%
20	4.298	917	920	923	rVB2	239	148	0.01%	0.001%
21	4.340	923	933	936	rBV2	222	334	0.02%	0.003%
22	4.359	936	939	942	rBV2	201	136	0.01%	0.001%
23	4.436	960	963	965	rBV	136	107	0.01%	0.001%
24	4.481	973	977	982	rVB2	219	209	0.01%	0.002%
25	4.523	987	990	993	rVB2	183	96	0.01%	0.001%
26	4.549	994	998	1000	rBV	124	109	0.01%	0.001%
27	4.645	1014	1028	1078	rBV	119876	464251	27.89%	3.956%
28	5.060	1140	1157	1185	rBV	264070	620550	37.28%	5.288%
29	5.189	1194	1197	1198	rBV2	381	220	0.01%	0.002%
30	5.250	1213	1216	1218	rBV	306	156	0.01%	0.001%
31	5.349	1245	1247	1248	rBV	426	198	0.01%	0.002%
32	5.362	1248	1251	1255	rVV2	381	406	0.02%	0.003%
33	5.420	1266	1269	1273	rBV	172	117	0.01%	0.001%
34	5.452	1277	1279	1282	rBV2	129	107	0.01%	0.001%
35	5.478	1284	1287	1289	rVB2	274	164	0.01%	0.001%
36	5.510	1295	1297	1300	rVB	226	108	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050505.D
 Acq On : 29 Aug 2022 23:52
 Operator : SY/MD
 Sample : N4344-19ME
 Misc : 5.85g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVR6ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

37	5.530	1300	1303	1306	rVB	257	122	0.01%	0.001%
38	5.575	1312	1317	1319	rBV	305	181	0.01%	0.002%
39	5.632	1333	1335	1339	rBV	159	86	0.01%	0.001%
40	5.716	1340	1361	1397	rVV2	658508	1664375	100.00%	14.182%
41	5.983	1432	1444	1468	rBV4	12796	33267	2.00%	0.283%
42	6.108	1481	1483	1486	rVB3	391	140	0.01%	0.001%
43	6.128	1487	1489	1494	rVB2	255	144	0.01%	0.001%
44	6.153	1494	1497	1501	rBV2	275	200	0.01%	0.002%
45	6.247	1508	1526	1551	rBV	464890	937643	56.34%	7.989%
46	6.533	1603	1615	1628	rBV8	5647	12176	0.73%	0.104%
47	6.603	1629	1637	1649	rVV3	5971	12719	0.76%	0.108%
48	6.690	1650	1664	1690	rVB	364233	754298	45.32%	6.427%
49	6.928	1735	1738	1741	rBV2	142	108	0.01%	0.001%
50	6.973	1748	1752	1756	rVV4	282	266	0.02%	0.002%
51	7.095	1788	1790	1794	rVB2	194	127	0.01%	0.001%
52	7.192	1813	1820	1821	rBV2	969	933	0.06%	0.008%
53	7.230	1823	1832	1845	rVB7	5234	11327	0.68%	0.097%
54	7.407	1884	1887	1891	rBB	299	176	0.01%	0.001%
55	7.433	1892	1895	1897	rBV	162	97	0.01%	0.001%
56	7.449	1897	1900	1904	rVB2	313	238	0.01%	0.002%
57	7.501	1913	1916	1921	rVB3	756	649	0.04%	0.006%
58	7.568	1921	1937	1958	rBV2	132765	262937	15.80%	2.240%
59	7.790	2003	2006	2007	rBV2	456	258	0.02%	0.002%
60	7.832	2016	2019	2024	rVB3	605	440	0.03%	0.004%
61	7.899	2024	2040	2061	rBV	659035	1204567	72.37%	10.264%
62	8.105	2102	2104	2106	rVB	432	189	0.01%	0.002%
63	8.182	2116	2128	2151	rBV2	85388	170736	10.26%	1.455%
64	8.314	2167	2169	2172	rBV3	269	150	0.01%	0.001%
65	8.349	2177	2180	2188	rVV4	1082	1413	0.08%	0.012%
66	8.552	2231	2243	2260	rVB	102519	175574	10.55%	1.496%
67	8.661	2260	2277	2309	rBV3	337396	932961	56.05%	7.950%
68	9.015	2384	2387	2388	rBV2	362	191	0.01%	0.002%
69	9.060	2399	2401	2408	rBV2	307	306	0.02%	0.003%
70	9.089	2408	2410	2411	rBV2	234	87	0.01%	0.001%
71	9.099	2411	2413	2418	rVB2	389	300	0.02%	0.003%
72	9.160	2429	2432	2436	rBV2	228	172	0.01%	0.001%
73	9.304	2475	2477	2482	rVB2	249	170	0.01%	0.001%
74	9.333	2483	2486	2492	rBV3	253	233	0.01%	0.002%
75	9.362	2492	2495	2498	rBV	369	250	0.02%	0.002%
76	9.420	2499	2513	2547	rBV	599718	1125274	67.61%	9.588%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050505.D
 Acq On : 29 Aug 2022 23:52
 Operator : SY/MD
 Sample : N4344-19ME
 Misc : 5.85g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVR6ME

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\SFAMULM082422WMA.M
 Title : VOC Analysis

77	9.607	2569	2571	2574	rBV2	439	236	0.01%	0.002%
78	9.738	2609	2612	2614	rBV	195	103	0.01%	0.001%
79	9.751	2614	2616	2620	rVB2	287	208	0.01%	0.002%
80	9.822	2634	2638	2640	rBV2	299	229	0.01%	0.002%
81	9.915	2664	2667	2668	rBV	238	129	0.01%	0.001%
82	9.973	2682	2685	2686	rBV	352	190	0.01%	0.002%
83	10.349	2800	2802	2804	rVB	231	95	0.01%	0.001%
84	10.378	2808	2811	2813	rBV	164	102	0.01%	0.001%
85	10.488	2842	2845	2847	rBV2	365	232	0.01%	0.002%
86	10.529	2855	2858	2860	rBV2	185	139	0.01%	0.001%
87	10.552	2863	2865	2869	rVB	331	167	0.01%	0.001%
88	10.600	2877	2880	2882	rBV	521	356	0.02%	0.003%
89	10.652	2892	2896	2898	rBV	531	365	0.02%	0.003%
90	10.764	2916	2931	2958	rBV	505113	861212	51.74%	7.338%
91	10.886	2966	2969	2970	rBV	456	235	0.01%	0.002%
92	10.960	2989	2992	2993	rBV	191	115	0.01%	0.001%
93	11.118	3037	3041	3049	rVB4	1733	1915	0.12%	0.016%
94	11.163	3051	3055	3058	rBV2	350	290	0.02%	0.002%
95	11.333	3105	3108	3112	rVB2	285	159	0.01%	0.001%
96	11.684	3214	3217	3219	rBV	368	202	0.01%	0.002%
97	11.754	3233	3239	3245	rBV2	1000	1322	0.08%	0.011%
98	11.815	3246	3258	3275	rBV	534342	853097	51.26%	7.269%
99	12.198	3364	3377	3394	rBV	567377	930523	55.91%	7.929%
100	12.909	3595	3598	3599	rBV2	478	234	0.01%	0.002%

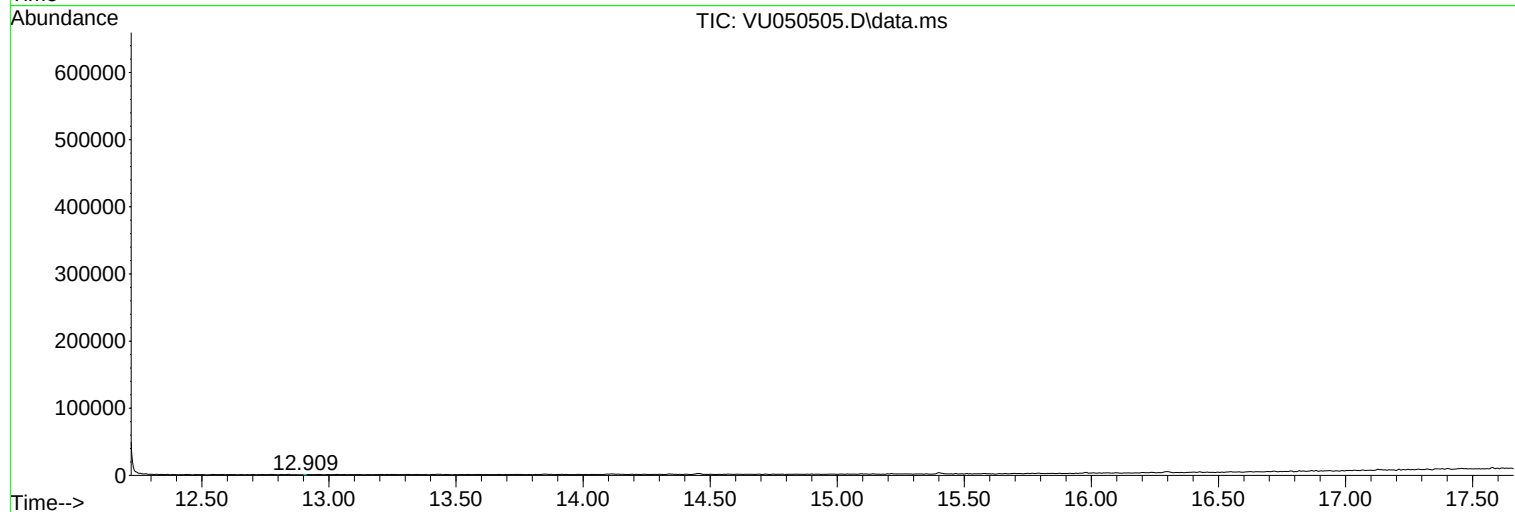
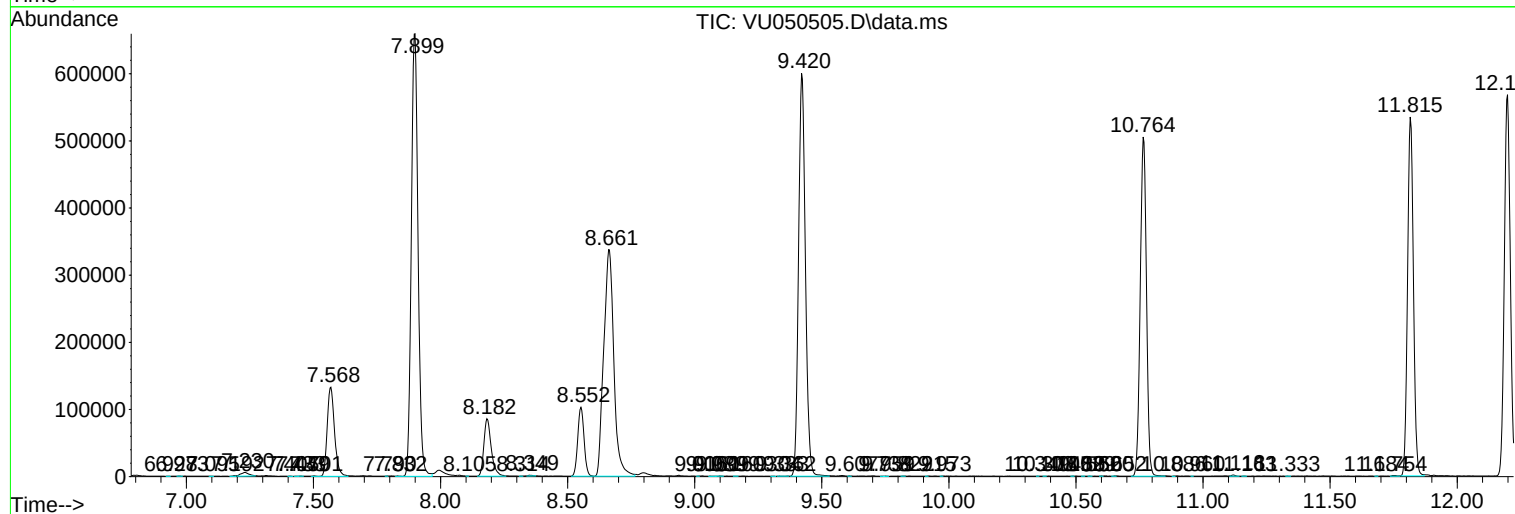
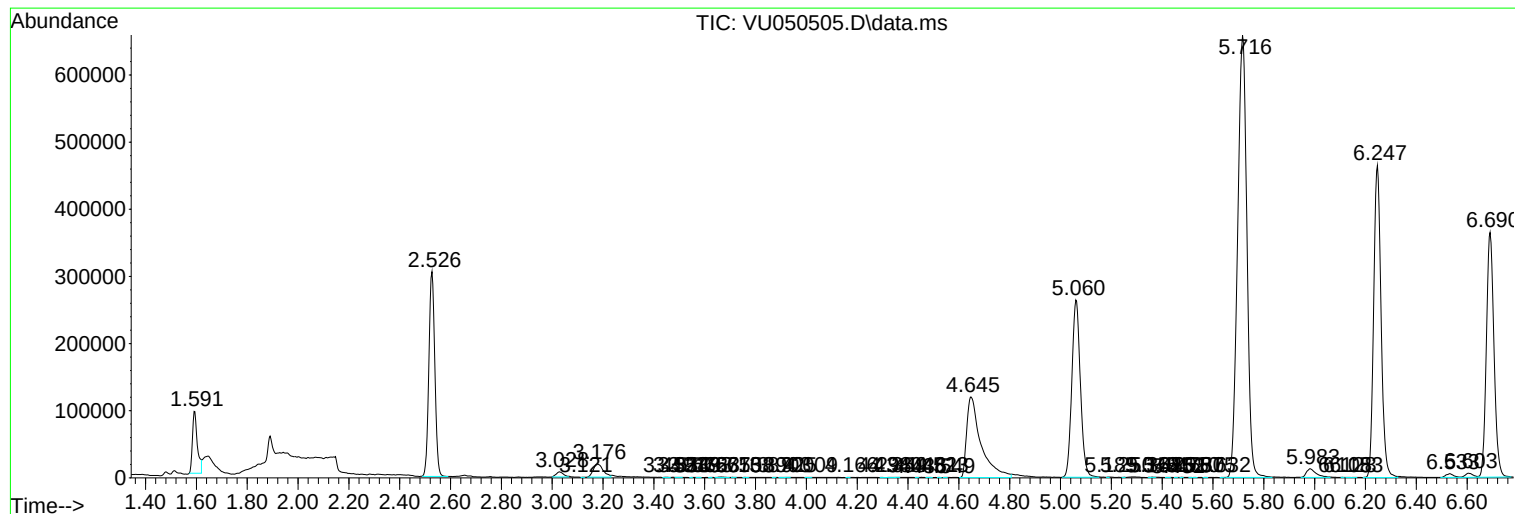
Sum of corrected areas: 11735974

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050505.D
Acq On : 29 Aug 2022 23:52
Operator : SY/MD
Sample : N4344-19ME
Misc : 5.85g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVR6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
Data File : VU050505.D
Acq On : 29 Aug 2022 23:52
Operator : SY/MD
Sample : N4344-19ME
Misc : 5.85g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVR6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.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\VU082922\
Data File : VU050505.D
Acq On : 29 Aug 2022 23:52
Operator : SY/MD
Sample : N4344-19ME
Misc : 5.85g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVR6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.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
------------------	----	---------	-------	----------	---	----	------	------