

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050536.D
 Acq On : 30 Aug 2022 23:38
 Operator : SY/MD
 Sample : N4363-08ME
 Misc : 6.03g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVW3ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050536.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	38	44	49	rBV2	4635	5781	0.19%	0.025%
2	1.510	49	53	59	rBV	4440	5674	0.19%	0.025%
3	1.594	71	79	87	rBV	181575	248693	8.15%	1.093%
4	1.883	163	169	179	rBV	82346	116781	3.83%	0.513%
5	2.533	357	371	393	rBV	577582	931280	30.54%	4.092%
6	2.751	434	439	441	rBV3	641	513	0.02%	0.002%
7	2.874	466	477	480	rBV3	909	1430	0.05%	0.006%
8	3.031	516	526	538	rVB2	11527	21702	0.71%	0.095%
9	3.115	550	552	556	rVB3	346	256	0.01%	0.001%
10	3.179	556	572	598	rBV2	33525	93018	3.05%	0.409%
11	3.401	638	641	646	rVB4	367	276	0.01%	0.001%
12	3.575	691	695	698	rBV2	330	312	0.01%	0.001%
13	3.671	719	725	728	rBV4	1064	1246	0.04%	0.005%
14	3.861	779	784	791	rVB3	334	388	0.01%	0.002%
15	3.896	791	795	797	rBV2	429	353	0.01%	0.002%
16	4.047	838	842	846	rBV	313	246	0.01%	0.001%
17	4.269	904	911	915	rVB2	216	271	0.01%	0.001%
18	4.417	953	957	960	rBV	275	228	0.01%	0.001%
19	4.639	1012	1026	1101	rBV	241458	829940	27.21%	3.647%
20	4.903	1106	1108	1111	rVV3	611	445	0.01%	0.002%
21	4.925	1111	1115	1121	rVB4	621	566	0.02%	0.002%
22	4.989	1132	1135	1139	rBV2	304	264	0.01%	0.001%
23	5.060	1139	1157	1188	rVV	503486	1151925	37.77%	5.062%
24	5.288	1219	1228	1238	rVB5	1421	2549	0.08%	0.011%
25	5.366	1249	1252	1260	rVB4	907	1128	0.04%	0.005%
26	5.510	1294	1297	1300	rBV2	286	262	0.01%	0.001%
27	5.591	1317	1322	1325	rBV2	303	312	0.01%	0.001%
28	5.716	1338	1361	1399	rBV2	1191228	3049632	100.00%	13.400%
29	5.980	1432	1443	1458	rVV5	9751	22818	0.75%	0.100%
30	6.247	1511	1526	1561	rBV	854057	1673063	54.86%	7.352%
31	6.526	1604	1613	1626	rBV	5673	11911	0.39%	0.052%
32	6.603	1626	1637	1649	rBV3	4427	10021	0.33%	0.044%
33	6.690	1649	1664	1691	rVV	689564	1382639	45.34%	6.075%
34	6.838	1707	1710	1712	rVB3	806	303	0.01%	0.001%
35	6.954	1743	1746	1751	rBV2	398	315	0.01%	0.001%
36	7.041	1767	1773	1776	rBV2	237	278	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050536.D
 Acq On : 30 Aug 2022 23:38
 Operator : SY/MD
 Sample : N4363-08ME
 Misc : 6.03g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVW3ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

37	7.140	1802	1804	1808	rVB2	378	234	0.01%	0.001%
38	7.224	1813	1830	1847	rVB2	3853	12122	0.40%	0.053%
39	7.298	1847	1853	1855	rBV4	489	470	0.02%	0.002%
40	7.333	1862	1864	1866	rBV	497	246	0.01%	0.001%
41	7.568	1923	1937	1961	rBV	285378	540660	17.73%	2.376%
42	7.693	1973	1976	1990	rVB3	1342	2391	0.08%	0.011%
43	7.751	1990	1994	1998	rBV2	289	251	0.01%	0.001%
44	7.803	2007	2010	2014	rVB3	478	351	0.01%	0.002%
45	7.896	2025	2039	2062	rBV	1350076	2398260	78.64%	10.538%
46	8.073	2092	2094	2104	rVB4	1297	1342	0.04%	0.006%
47	8.182	2115	2128	2154	rVV	183830	359286	11.78%	1.579%
48	8.308	2165	2167	2171	rVB4	357	304	0.01%	0.001%
49	8.336	2171	2176	2177	rBV3	449	288	0.01%	0.001%
50	8.353	2178	2181	2185	rVV5	806	625	0.02%	0.003%
51	8.426	2198	2204	2205	rVV	435	389	0.01%	0.002%
52	8.455	2209	2213	2217	rVB3	271	278	0.01%	0.001%
53	8.552	2230	2243	2259	rBV	656567	1106873	36.30%	4.864%
54	8.655	2259	2275	2313	rVV3	763692	1784054	58.50%	7.839%
55	8.934	2360	2362	2367	rVB4	389	307	0.01%	0.001%
56	9.034	2390	2393	2396	rBV2	474	379	0.01%	0.002%
57	9.053	2397	2399	2404	rVV2	534	491	0.02%	0.002%
58	9.076	2404	2406	2409	rVV2	469	333	0.01%	0.001%
59	9.420	2499	2513	2545	rBV	1126228	2029788	66.56%	8.919%
60	9.574	2559	2561	2567	rVB5	888	753	0.02%	0.003%
61	9.693	2590	2598	2601	rBV3	774	985	0.03%	0.004%
62	9.880	2654	2656	2662	rVB2	500	316	0.01%	0.001%
63	9.906	2662	2664	2667	rBV2	311	230	0.01%	0.001%
64	9.967	2678	2683	2686	rVB2	446	416	0.01%	0.002%
65	10.095	2719	2723	2726	rBV2	349	293	0.01%	0.001%
66	10.131	2731	2734	2738	rVB3	454	403	0.01%	0.002%
67	10.253	2767	2772	2774	rBV	324	261	0.01%	0.001%
68	10.291	2780	2784	2788	rBV3	285	280	0.01%	0.001%
69	10.449	2827	2833	2835	rBV2	449	389	0.01%	0.002%
70	10.590	2874	2877	2880	rBV2	423	234	0.01%	0.001%
71	10.610	2881	2883	2886	rBV	353	271	0.01%	0.001%
72	10.648	2892	2895	2897	rBV3	386	277	0.01%	0.001%
73	10.764	2916	2931	2951	rBV	1008748	1667042	54.66%	7.325%
74	10.873	2961	2965	2969	rVB2	462	415	0.01%	0.002%
75	11.021	3009	3011	3015	rVB2	419	251	0.01%	0.001%
76	11.114	3035	3040	3054	rVB4	1881	2420	0.08%	0.011%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050536.D
 Acq On : 30 Aug 2022 23:38
 Operator : SY/MD
 Sample : N4363-08ME
 Misc : 6.03g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVW3ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

77	11.327	3103	3106	3112	rVB3	359	385	0.01%	0.002%
78	11.388	3119	3125	3126	rBV	421	411	0.01%	0.002%
79	11.417	3131	3134	3142	rBV3	416	460	0.02%	0.002%
80	11.539	3169	3172	3177	rBV2	347	248	0.01%	0.001%
81	11.684	3213	3217	3220	rVB3	424	350	0.01%	0.002%
82	11.815	3245	3258	3283	rBV	944900	1484064	48.66%	6.521%
83	12.147	3356	3361	3363	rBV	518	456	0.01%	0.002%
84	12.195	3363	3376	3398	rBV	1110570	1782769	58.46%	7.834%
85	12.446	3451	3454	3459	rVB2	393	239	0.01%	0.001%
86	12.513	3472	3475	3482	rBV2	284	365	0.01%	0.002%
87	12.886	3586	3591	3593	rBV2	411	391	0.01%	0.002%
88	13.102	3654	3658	3662	rBV2	528	503	0.02%	0.002%
89	13.134	3666	3668	3673	rVB2	379	268	0.01%	0.001%
90	13.233	3696	3699	3704	rVB3	683	614	0.02%	0.003%
91	13.391	3745	3748	3749	rBV2	349	240	0.01%	0.001%
92	13.449	3762	3766	3770	rBV	482	458	0.02%	0.002%
93	13.854	3888	3892	3898	rVB4	894	847	0.03%	0.004%
94	13.986	3930	3933	3937	rBV3	438	397	0.01%	0.002%
95	14.336	4039	4042	4049	rVB3	661	723	0.02%	0.003%
96	14.391	4056	4059	4062	rBV2	539	450	0.01%	0.002%
97	14.626	4130	4132	4135	rBV2	387	237	0.01%	0.001%
98	14.677	4145	4148	4151	rBV	435	317	0.01%	0.001%
99	14.847	4199	4201	4204	rBV2	481	291	0.01%	0.001%
100	14.902	4214	4218	4219	rBV2	522	392	0.01%	0.002%

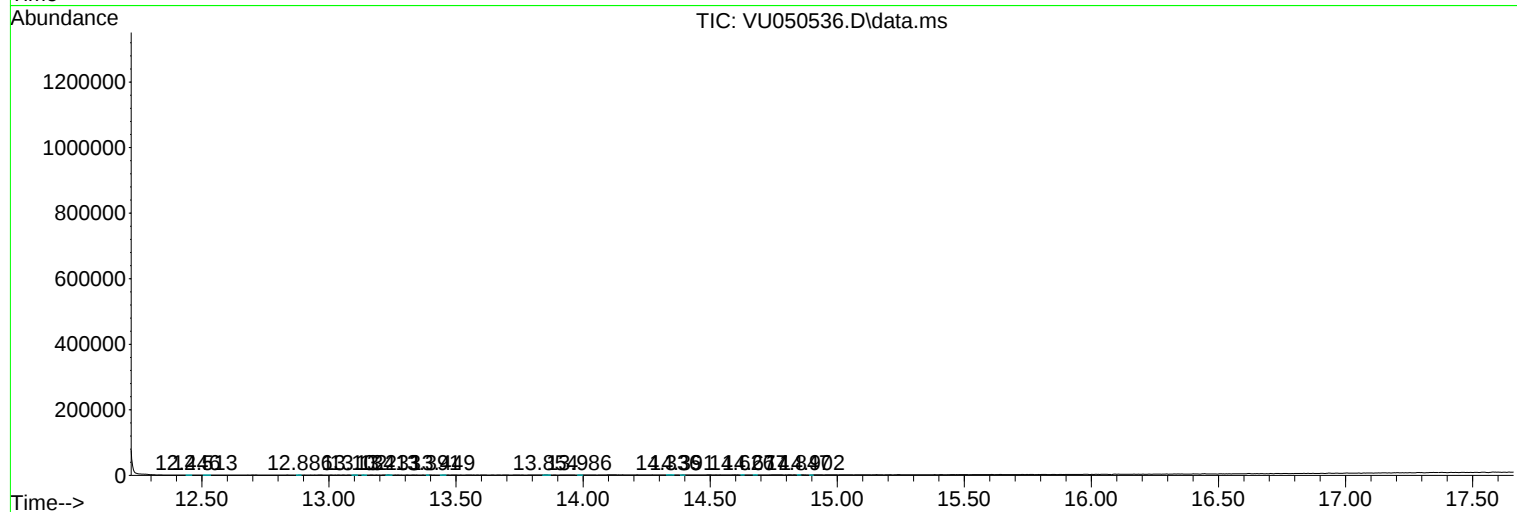
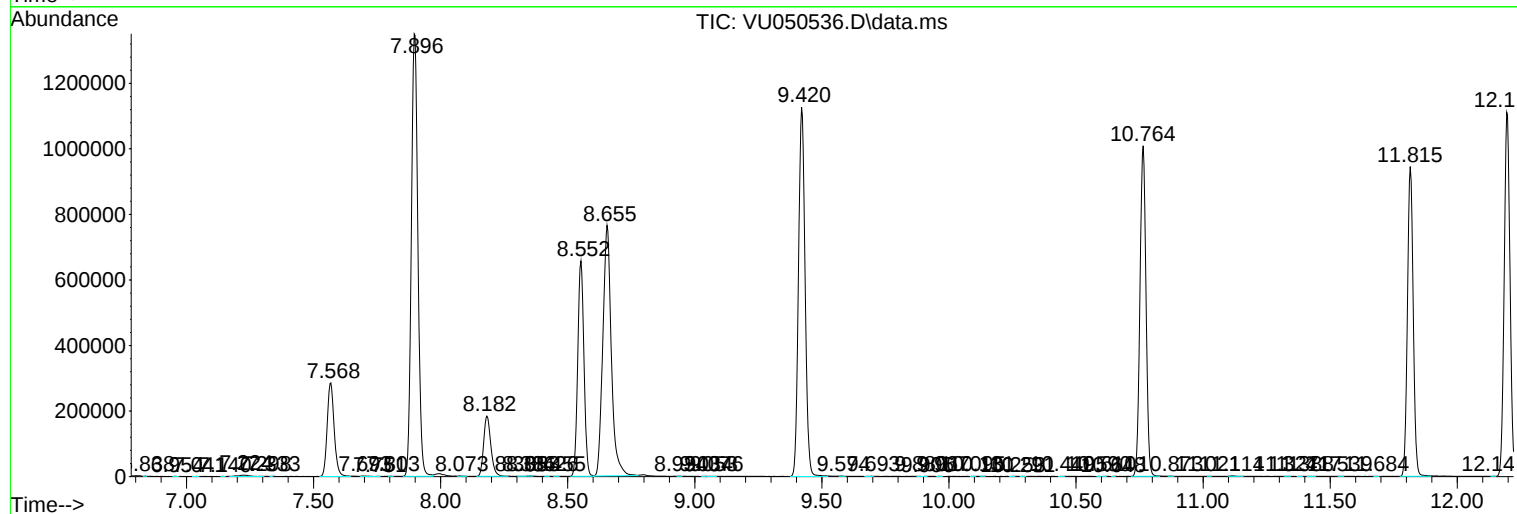
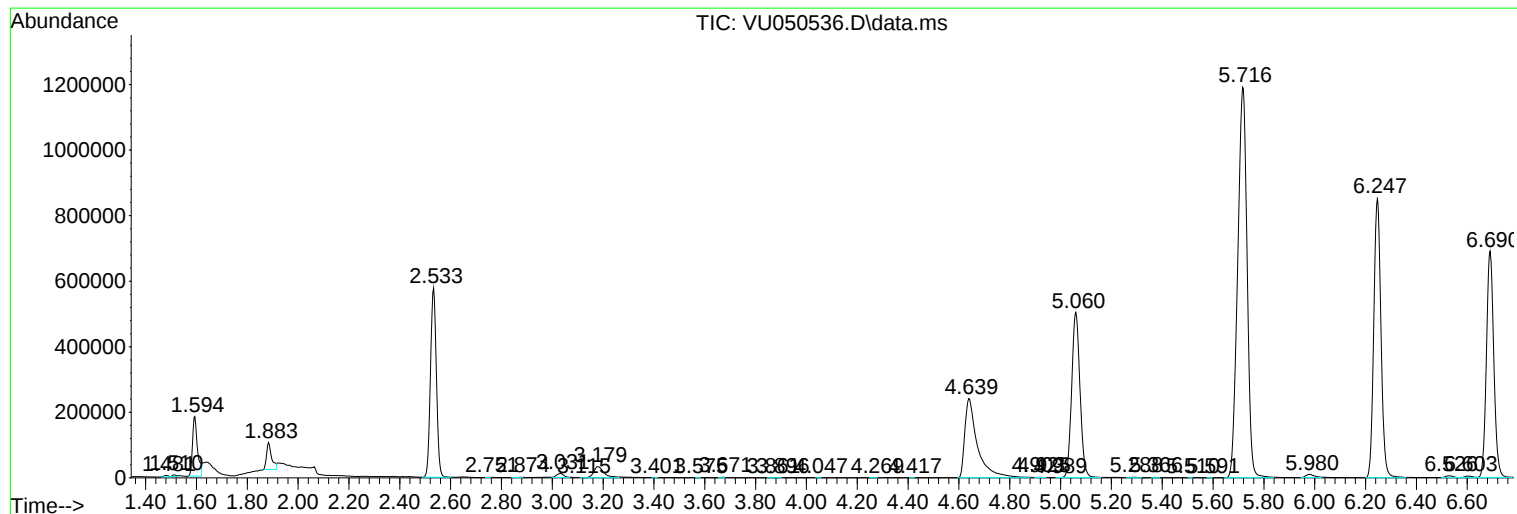
Sum of corrected areas: 22757652

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
Data File : VU050536.D
Acq On : 30 Aug 2022 23:38
Operator : SY/MD
Sample : N4363-08ME
Misc : 6.03g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVW3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
Data File : VU050536.D
Acq On : 30 Aug 2022 23:38
Operator : SY/MD
Sample : N4363-08ME
Misc : 6.03g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVW3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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\VU083022\
Data File : VU050536.D
Acq On : 30 Aug 2022 23:38
Operator : SY/MD
Sample : N4363-08ME
Misc : 6.03g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVW3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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